Heat Capacity of Liquids: Critical Review and Recommended Values. Supplement II

Cite as: J. Phys. Chem. Ref. Data **39**, 013103 (2010); https://doi.org/10.1063/1.3182831
Submitted: 21 April 2008 . Accepted: 29 June 2009 . Published Online: 31 March 2010

Milan Zábranský, Zdenka Kolská, Vlastimil Růžička, and Eugene S. Domalski

Heat Capacity of Liquids: Critical Review and Recommended Values. Supplement II

Milan Zábranský
Department of Physical Chemistry, Institute of Chemical Technology, 166 28 Prague 6, Czech Republic

Zdenka Kolská
Department of Chemistry, Faculty of Science, J. E. Purkinje University, České mládeže 8, 400 96 Ústí nad Labem, Czech Republic

Vlastimil Růžička, Jr.[a)]
Department of Physical Chemistry, Institute of Chemical Technology, 166 28 Prague 6, Czech Republic

Eugene S. Domalski
National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

(Received 21 April 2008; accepted 29 June 2009; published online 31 March 2010)

A study was carried out in which new experimental data on heat capacities of pure liquid organic and some inorganic compounds were compiled and critically evaluated and recommended values provided. The bulk of the compiled data covers data published in the primary literature between 2000 and 2006 and includes some data published in 2007. However, some data from older sources are also included. The list of compound families covered was extended to include ionic liquids. Parameters of correlating equations for the temperature dependence of heat capacities of liquids were developed. This paper is an update of a two volume monograph entitled *Heat Capacity of Liquids: Critical Review and Recommended Values* by Zábranský *et al.* [J. Phys. Chem. Ref. Data 30, 1199 (2001)], which was published in 1996 in the Journal of Physical and Chemical Reference Data as Monograph No. 6, and of Supplement I. *© 2010 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [doi:10.1063/1.3182831]

Key words: bibliography; collections of physical data; correlating equations; critically evaluated data; heat capacity; liquids; specific heat; organic compounds.

CONTENTS

[a)]Electronic mail: vlastimil.ruzicka@msmt.cz.

List of Tables

List of Figures

1. Introduction

Heat capacities are among the basic thermophysical and thermodynamic properties which characterize a liquid. They are directly linked with temperature derivatives of basic thermodynamic functions and are therefore indispensable for the calculation of differences in these functions at different temperatures. This information is widely used in chemical engineering for establishing energy balances, in thermodynamics for obtaining entropy and enthalpy values, and in thermochemistry for calculating changes in reaction enthalpies with temperature. A knowledge of heat capacities is also required for evaluating the effect of temperature on phase and reaction equilibria. Variations in heat capacities serve as a sensitive indicator of phase transitions and are an important tool for understanding changes in the structure of liquid solutions.

This paper includes new data on heat capacities for 205 compounds not included in Monograph No. 6 (1996ZAB/RUZ) or in Supplement I (2001ZAB/RUZ). The list of fami-

lies of compounds covered was extended by ionic liquids, a group of compounds that has received large attention over the past several years. Also included are new data that either extend the temperature range of recommended data for compounds already presented in the two works cited above or improve the overall uncertainty of the recommended data by supplying new data that have a lower error of measurement; this pertains to more than 150 compounds. Finally, references to new data for about 80 compounds are simply presented in a review of primary sources where new measurements do not extend or improve the previously developed recommended data.

The objectives of the present study are as follows:

(i) To provide an exhaustive survey of the literature for all isobaric and saturation heat capacities for pure organic and inorganic compounds in the liquid state which were published in the primary literature mainly between 2000 and 2006 and some data of 2007. Only data for well-defined compounds in the isotropic liquid state, obtained by calorimetric measurements, were considered. The criterion for inclusion of a compound in the compilation required the compound to have a melting point below 573 K.
(ii) To compile newly published heat capacities and to extend a computer readable database of raw experimental data established in previous projects.
(iii) To critically evaluate heat capacity data and prepare sets of selected data.
(iv) To correlate selected data and provide recommended values for the heat capacities of liquid compounds as a function of temperature. The recommended data are presented in terms of parameters of suitable correlating equations accompanied with an assessment of the data uncertainty.

In this paper we utilized some material from the textual part of Monograph No. 6 (1996ZAB/RUZ) which is necessary for describing the compilation, critical assessment and correlation of data as well as for understanding the tables. The text was updated where needed and/or new information was added.

2. Calorimetric techniques for determining heat capacities of liquids

2.1. Terminology and criteria for classification of calorimeters

The type of the calorimeter used for obtaining the experimental data is one of the most important criteria for judging the quality of the data. As there is no officially established nomenclature for describing different types of calorimeters we used the terminology was proposed by Zábranský *et al.* (1996ZAB/RUZ) for classifying calorimeters. Some basic ideas of this classification are described in this section.

Heat capacity calorimeters can be classified according to four criteria:

(1) *motion of the sample inside the instrument* (batch, flow, and drop calorimeters),
(2) *mode of measurement* (stationary or dynamic conditions),
(3) *temperature relationship between the calorimeter vessel and its surroundings—mode of heat transfer* (adiabatic, isoperibol, isothermal, and conduction calorimeters), and
(4) *number of calorimeter vessels* (single vessel and twin vessel calorimeters).

Table 1 lists individual criteria with the codes used for characterizing calorimeters in Tables 2 and 3 and in tables with experimental values. It should be kept in mind that the codes serve for a concise categorization of instruments and the adopted system of classification does not pretend to be exhaustive.

2.2. Survey of calorimeters

TABLE 1. Criteria codes used for classification of calorimeters

Motion of Sample 1		Mode of Measurement 2		Temperature Relation of Vessel to Surroundings 3		Number of Vessels 4	
batch	B	stationary	S	adiabatic	A	one vessel	O
flow	F	dynamic	D	isoperibol	I	two vessels	T
drop	D			isothermal	T		
				conduction	H		
				thermopile conduction	C		

TABLE 2. Types of calorimeters used for determining heat capacities

	Classification			
Type of Calorimeter	1	2	3	4
Adiabatic batch calorimeters with intermittent heating	B	S	A	O
Adiabatic batch calorimeters with continuous heating	B	D	A	O
Isoperibol batch calorimeters	B	S	I	O/T
Isoperibol flow calorimeters	F	S	I	O/T
Isoperibol drop calorimeters	D	S	I	O
Adiabatic drop calorimeters	D	S	A	O
Isothermal drop (phase change) calorimeters	D	S	T	O
Thermopile conduction drop calorimeters	D	D	C	T
Measurements of heating and/or cooling curves	B	D	H	O
Differential heat conduction calorimeters (TA, DTA, DSC)	B	D	H	T
Differential thermopile-conduction calorimeters	B	D	C	T
Special dynamic methods using pulse techniques	B	D	H	O

TABLE 3. Survey of calorimeters for determining heat capacity

Reference	Temperature Range	Measurement Error	Note
Adiabatic batch calorimeters with intermittent heating			
1920COH/MOE	room	medium	
1924WIL/DAN	300–360 K	medium	
1930SOU/AND	low	0.50%	
1933SOU/BRI	low	high	
1935AOY/KAN	low	medium	
1939AST/EID1	low	high	
1939SAG/EVA	300–370 K	2.00%	high pressure, also for heat of vaporization
1943RUE/HUF	low	0.10%	
1944BAI/TOD	80–340 K	1.00%	
1945SCO/MEY	low	0.10%	
1947HUF	low	0.10%	detailed description of improvements in calorimeter, 1943RUE/HUF
1947OSB/GIN	medium	0.10%	also for heat of vaporization
1947SKU	room	0.30%	
1949STA/GUP	low	medium	
1950SAG/HOU	medium and high	1.00%	high pressure (up to 6.9 MPa)
1951EUC/EIG	medium	medium	
1952ADA/JOH	low and medium	high	
1953WES/HAT	250–550 K	0.15%	
1954STR/ICK	low	0.30%	
1955STA/TUP	283–373 K	1.00%	
1956POP/KOL	60–300 K	0.50%	
1957PIL	low and medium	medium	
1958HIL/KRA	low	0.30%	
1958WES/GIN	303–773 K	0.10%	
1959ONK	293–373 K	high	
1961GOO	low	high	high pressure
1961ROU	283–323 K	medium	
1963AND/COU1	low	high	
1963BEN	273–343 K	high	
1964ARN1	293–453 K	0.30%	
1965STE/BLA	10–360 K	0.10%	
1965SUG/SEK	15–310 K	0.30%	
1966KLE	293–343 K	high	
1966NIK/LEB	60–300 K	0.30%	
1967RAS/GAN	298–473 K	0.50%	
1968CLE/MEL	80–320 K	high	
1968REC1	room	medium	
1968WES/FUR	low	high	
1968WES/WES	300–800 K	high	
1971GOP/GAM	303–343 K	1.00%	
1972VAN	123–373 K	high	
1974ATA/CHI	2–300 K	high	
1974DIA/REN	medium	0.30%	
1974MOS/MOU	273–346 K	low	
1975VYU/ZVE	medium	high	
1976LEB/LIT	5–340 K	0.30%	measurement error: 3%–5% below 20 K, 0.5%–1% between 20 and 60 K, 0.15%–0.3% above 60 K
1977KU/COM	low	1.00%	
1977NAZ/MUS	293–620 K	1.50%	high pressure (up to 50 MPa)
1977VOR/PRI	room	high	
1978SOL/SUK	123–283 K	medium	also for heat of vaporization
1978ZHU/ATR	medium	medium	commercial instrument made by VNIIFTRI (Khabarovsk)
1979AMI/LEB	5–300 K	high	
1979SCH/OFF	90–350 K	high	
1979VES/ZAB	293–318 K	0.50%	

TABLE 3. Survey of calorimeters for determining heat capacity—Continued

Reference	Temperature Range	Measurement Error	Note
1980KAL/JED	90–300 K	0.10%	
1980SHA/LYU	15–330 K	0.50%	
1980VAS/TRE	313–623 K	low	
1983KUK/KOR	263–353 K	0.20%	
1983YOS/SOR1	15–390 K	0.20%	
1985RAB/SHE	low	0.30%	measurement error: 1.8% below 10 K, 0.8% between 10 and 25 K, 0.3% above 30 K
1987VAN/VAN	10–350 K	0.20%	
1987YAM/OGU	12–370 K	0.30%	high pressure (up to 250 MPa)
1988STE/ARC	low and medium	0.10%	modification of the calorimeter originally described by 1943RUE/HUF and 1947HUF
1991SVO/ZAB1	293–353 K	0.30%	also for heat of vaporization
1992SOR/KAJ	13–530 K	0.25%	
1993DIK/KAB	5–305 K	0.40%	commercial instrument TAU-1 made by VNIFTRI (Moscow); the error at helium temperatures is 2% at decreased to 0.4% at 40 K
1993FUJ/OGU1	2–400 K	0.20%	inaccuracy to be within 0.3% and 0.2% below and above 35 K, respectively
1995TAN/SUN	60–350 K	0.50%	
1997VAR/DRU1	5–350 K	0.20%	instrument made by VNIIFTRI (Mendeleevo)
1998VAN/VAN	5–400 K	0.20%	
1999TAN/ZHA	80–400 K	0.20%	
2002VAN/VAN1	10–420 K	0.50%	for small volume of sample (0.6 ccm)
	Adiabatic batch calorimeters with continuous heating		
1931DEE	low	medium	
1951POP/GAL	300–1000 K	medium	
1965FIN/GRU	room	0.40%	
1971MUS	293–773 K	2.50%	high pressure (up to 50 MPa)
1975RAS/GRI	medium and high	1.00%	high pressure
1987OKH/RAZ	medium	0.30%	
	Isoperibol batch calorimeters		
1907BAT	low	low	
1909SCH	medium	low	
1912SCH1	medium	low	
1913CAM	medium	low	
1919DEJ	medium	low	
1920GIB/LAT	low and medium	low	
1925DRU/WEI	room	low	
1925PAR	low	0.50%	
1928LAT/GRE	low	medium	
1929KEL1	low	medium	
1929MIT/HAR1	low	medium	
1931BLA/LEI	medium and high	3.00%	
1931FIO/GIN	medium and high	high	also for heat of vaporization
1932NEU	medium	medium	
1933LEB/MOE	room	medium	
1934LON/REY	300–560 K	low	
1935JAC	medium	medium	
1936GIA/STO	low	0.20%	
1937ELL	medium	medium	
1937GIA/EGA	low	high	measurement error: 3% at 15 K, 1% at 20 K, 0.2% above 35 K
1937VOL	room	low	
1939MAZ3	low and medium	low	
1943BAC/PER	medium	medium	
1948TSC1	room	low	also for heat of mixing

TABLE 3. Survey of calorimeters for determining heat capacity—Continued

Reference	Temperature Range	Measurement Error	Note
1949TSC/RIC1	room	medium	also for heat of mixing
1949WEI	room	low	
1952STA/AMI	medium	low	also for heat of vaporization
1955HUT/MAN	297–299 K	medium	
1955RUI1	room	medium	also for heat of mixing
1957CRU/JOS	medium	2.00%	
1957KEN	medium	1.00%	also for heat of mixing
1958MUR/VAN	room	2.35%	
1959BAK	300–353 K	high	
1962KAT	medium	medium	
1964MOE/THO	293–313 K	low	
1964RAS/BAS	medium	1.50%	
1966DRA/LAN	room	medium	
1966SAV	293–333 K	1.20%	
1967GRA	303–338 K	1.00%	
1970LKB/COM	278–333 K	medium	
1970REC	room	medium	
1975PED/KAY	medium	1.00%	
1976BON/CER	room	medium	
1978RYB/EME	medium	low	
1979CZA	room	low	high pressure (up to 1000 MPa)
1980FUC	293–300 K	0.50%	
1983MEY/MEY	medium	medium	
1988ROD/MAR	room	medium	commercial instrument Tronac model 458
1998HAW/GRA	298–298 K	medium	commercial instrument Hart 4285
		Isoperibol batch calorimeters	
1934KOL/UDO2	room	low	
1939BYK	298–305 K	low	
		Isoperibol flow calorimeters	
1928LAN	medium	medium	
1959RIB/EGO	293–573 K	medium	high pressure (up to 25 MPa)
1965KAU/BIT	293–350 K	1.00%	
1975SAF/GER	medium and high	0.60%	high pressure (up to 50 MPa)
1975SAN	293–573 K	0.60%	high pressure (up to 5 MPa)
1983GOR/SIM	medium	medium	
1985OGA	Room	0.10%	
1987LAN/CRI	high	medium	
1999BUR/ZOC	258–373 K	2.00%	multipurpose apparatus for excess enthalpy, heat capacity, density, kinematic viscosity and thermal conductivity
		Isoperibol differential flow calorimeters	
1971PIC/LED	room	medium	
1988CON/GIA	medium	medium	constructed according to Picker instrument (1971PIC/LED)
		Isoperibol drop calorimeters	
1879BER	medium	low	
1881VON	medium	medium	
1886LUD	medium	low	
1886SCH	medium	medium	
1894BRU	293–370 K	low	
1898LOU	medium	medium	
1901KAH	medium	low	
1907GUI2	high	medium	
1907WAL	room	low	pure solid metal dropped into liquid sample
1908BOG/WIN	medium	low	
1909GOO/KAL	high	medium	
1911LEW/RAN	293–663 K	low	

TABLE 3. Survey of calorimeters for determining heat capacity—Continued

Reference	Temperature Range	Measurement Error	Note
1912LUS	medium	low	
1918NAR	medium	low	
1922HER/SCH	Room	low	
1924GAR/RAN	medium	low	
1926AND/LYN	low and medium	low	
1933ROT/MEY2	273–628 K	medium	
1936KUR/VOS	room	low	
1947KUR	medium	low	estimated measurement error about 5%
1947PUS/FED	room	low	
1958GOO/SOL	high	1.00%	
1958SWI/ZIE1	medium	low	
1964CAM/NAG	medium and high	medium	
1971MAR/CIO	300–1300 K	low	
		Adiabatic drop calorimeters	
1930BAR/MAA	medium	1.00%	
		Isoperibol drop (phase change) calorimeters	
1916BRA	medium	0.40%	Bunsen ice calorimeter
1935BAR/CLU	medium	low	Bunsen ice calorimeter
1950GIN/DOU	273–1173 K	0.35%	Bunsen ice calorimeter
		Thermopile conduction drop calorimeters	
1971KON/SUU	273–343 K	0.10%	
1974SUU/WAD	273–343 K	high	
		Measurement of heating and/or cooling curve	
1890PIC	medium	low	
1931THO/PAR	293–773 K	low	
1933FER/MIL	293–323 K	1.00%	
1937STU	90–320 K	1.00%	
1940COC/FER	room	low	
1949WUY/JUN	medium	medium	
1950KUS/CRO	medium	1.50%	dielectric constant measured simultaneously
1959ABA/MUS	room	low	
1979TAK/YOK	80–1100 K	1.00%	
1981ATA/ELS	room	low	
1984FIL/LAU	medium	2.00%	
1986NAZ/BAS1	303–523 K	2.00%	high pressure (up to 50 MPa)
		Differential heat conduction calorimeters (TA, DTA, DSC)	
1963GUD/CAM	medium	low	
1966PER/COM	340–510 K	1.00%	
1968OST/DOB	290–473 K	medium	
1969PER/COM	medium and high	low	commercial calorimeter DSC-2; measurement error 1% above 200 K
1969YAG	200–670 K	2.50%	commercial instrument denoted as ADKTTM; triple-heat bridge method
1971DU/COM	room	low	
1973PER/COM	medium and high	low	
1979DU/COM	medium and high	low	
1981ARU	medium and high	1.50%	high pressure (up to 60 MPa)
1984GUS/MIR	303–523 K	2.00%	high pressure
1985GUS/DAV	150–700 K	2.50%	Instrument denoted as ADKTTM; triple-heat bridge method
1987PER/COM	medium and high	1.50%	commercial instrument Shimadzu model DSC-50
1989KNI/ARC	high	1.00%	commercial instrument Perkin-Elmer DSC-2
1989PRA/RAJ	318–333 K	3.00%	
1992HWA/DES	medium and high	low	commercial instrument Perkin-Elmer DSC-4
1992KAB/KOZ	340–520 K	1.50%	triple-heat bridge method

TABLE 3. Survey of calorimeters for determining heat capacity—Continued

Reference	Temperature Range	Measurement Error	Note
1993CON/GIR1	298–498 K	low	commercial instrument TA 2000 Mettler; used high pressure crucibles with a teflon membrane
1995DIO/MAN	medium and high	low	commercial instrument Perkin-Elmer DSC-7
1995MOR/IDR1	medium and high	1.00%	commercial instrument Seiko heat-flux DSC 220 system
1998MUT/WIL	273–373 K	low	commercial instrument TA Instrument Modulated DSC-2910
1998SAL/FER	medium	medium	modulated scanning calorimeter
1999CHI/LIU	medium	low	commercial instrument TA instrument DSC-2010 and TA controller
1999MO/YAN	medium	low	commercial instrument Perkin-Elmer PYRIS I
2001NGE/MAL	310–600 K	medium	commercial instrument Shimadzu DSC-50
2002VAN/VAN2	medium and high	medium	commercial calorimeter Mettler Toledo DSC821e
2002ZHA/HAW	medium	2.00%	heat flux CSC4100
2003YAN/MA1	medium	1.00%	commercial instrument Netzsch Producer, DSC-204 (Germany)
2004CHE/CLE	medium and high	1.50%	commercial instrument Netzsch DSC-404C
2004FRE/CRO	medium and high	5.00%	commercial instrument Mettler Toledo DSC822
2004KIM/SHI	medium	medium	commercial instrument TA DSC Q100
2004YAN/MA	medium	2.00%	commercial instrument Netzsch Producer, DS4-204 Phoenix
2005FUJ/MAT	medium	medium	commercial instrument DSC Calorimetry Science Corp. USA CSC5100
		Differential thermopile conduction calorimeters	
1965STE/CAL	medium	medium	
1968WAD	medium	medium	commercial instrument LKB-8700; for heat of mixing
1970PAZ/PAZ	medium	medium	modified commercial SETARAM microcalorimeter
1974PET/TER	298–475 K	1.00%	
1976CON/GIA	medium	medium	
1978BYV/JAS	medium	2.00%	
1982ZAR	medium	medium	
1983ROU/ROU	278–368 K	high	modified commercial SETARAM microcalorimeter DSC
1986MER/BEN	150–1100 K	medium	commercial instrument SETARAM DSC 111
1989BRE/LIC	170–370 K	2.00%	commercial SETARAM microcalorimeter DSC 111 G
1991BAN/GAR	298–573 K	medium	commercial instrument SETARAM model C-80
1992FIL/AFA	283–353 K	medium	
2000BEC/AUF	77–473 K	0.30%	commercial SETARAM calorimeter (model BT2.15)
2000BES/SAI2	303–473 K	0.60%	modified commercial instrument SETARAM C80 with densimetr; for high pressure up to 100 MPa
2000ERN/CHO	medium	0.10%	commercial microcalorimeter SETARAM DSC-III
2004BOL/NER	medium	3.00%	instrument IT-CP-400 (Russia)
2007STR/RUZ	253–393 K	1.00%	commercial instrument SETARAM Micro DSC-III

3. Methodology of data treatment: establishment of recommended data

3.1. Database of raw values

The experimental values extracted from the literature together with auxiliary data were stored in the database of raw experimental values. The merged database containing both the data compiled in previous projects leading to Monograph No. 6 (1996ZAB/RUZ) and Supplement I (2001ZAB/RUZ) and the newly compiled data covers 2185 compounds and consists of 4789 data sets (set of experimental values from one calorimeter reported by an author for one substance in one original source). Only the parameters for smoothing equations are available for 354 data sets (no discrete data points were reported in these sources). The data sets of discrete values contain 43 134 raw data points. The auxiliary data comprise information on the quality of experimental values, sample purity and its determination, the nature of the experimental procedure (calorimetric technique and type of resulting heat capacity), the type of the measured heat capacities, and units used in the original source. This information was used later as a guide in the selection of data sets for the final correlation. Most auxiliary data are summarized for individual substances in tables of experimental heat capacities.

According to the information in the literature sources, we distinguished three types of heat capacities in the database of raw values: the *isobaric heat capacity* C_p,

$$C_p = T(\partial S/\partial T)_p = (\partial H/\partial T)_p = -T(\partial^2 G/\partial T^2)_p, \quad (1)$$

the *saturation heat capacity*

$$C_{\text{sat}} = T(\partial S/\partial T)_{\text{sat}}, \tag{2}$$

and the *average heat capacity* C_{avg},

$$C_{\text{avg}} = \frac{Q}{T_2 - T_1}. \tag{3}$$

Using well known thermodynamic relationships, one can derive conversion equations between the individual heat capacities. Among them, the most important for the present study is the relationship between the isobaric and saturation heat capacities

$$C_p - C_{\text{sat}} = T\frac{(\partial V/\partial T)_p}{(\partial p/\partial T)_{\text{sat}}}. \tag{4}$$

Below the normal boiling temperature T_{b} the measured isobaric heat capacity usually relates to atmospheric pressure though this is not frequently specified in the original source. C_p has limited dependence on pressure at low and moderate vapor pressures, and its effect can be neglected unless the pressure change is large. Below the normal boiling temperature no distinction was made between the literature C_p data relating to the saturation line, to atmospheric conditions, or to 101.325 kPa; these were considered as identical. Above the normal boiling temperature, the saturation heat capacities C_{sat} rather than C_p data are reported in the original literature.

3.2. Evaluation and selection process

All available sources were critically assessed. The important part of the selection process was the simultaneous correlation of all experimental data which served to test the consistency and helped reveal systematic errors. The correlation was performed by the weighted least-squares method; the minimized objective function S had the form

$$S = \sum_{i=1}^{n} \frac{(C_{\text{sm}} - C_{\text{exp}})^2}{\sigma^2 C_i}, \tag{5}$$

where the summation is over all the values included in the correlation and the subscripts "exp" and "sm" relate to experimental and smoothed values, respectively. The reciprocal of the *variance*, $\sigma^2 C$, is the *weighting factor*. It was estimated for each value on the basis of the assumed experimental error of the data set used in the correlation. The input information was the percentage error of the experimental data, $\sigma_{\text{r}} C$, as given by the author for the whole data set or estimated by the evaluator in cases where no information was available in the literature or the error assigned by the author/s was unrealistic. Thus the variance of the ith data point was expressed as

$$\sigma^2 C_i = \left(\frac{C_i \sigma_{\text{r}} C_i}{100}\right)^2. \tag{6}$$

The following criteria were observed in the selection process:

(i) accuracy of the experimental technique claimed by the author,
(ii) performance history of the laboratory,
(iii) consistency of the data with the values from other sources (if available),
(iv) purity of the substance,
(v) type of the calorimeter,
(vi) date of data origin, and
(vii) scatter of the data.

Selection and correlation of data for each compound were carried out simultaneously as described in 1996ZAB/RUZ and 2001ZAB/RUZ. The main criterion for judging the quality of the correlation was the *standard weighted deviation* s_{w}:

$$s_{\text{w}} = \left(\frac{S_{\min}}{n - m}\right)^{1/2}, \tag{7}$$

where $S_{\min}$ is the value of the objective function at its minimum, n is the overall number of the fitted data points, and m is number of independent adjustable parameters in a correlation equation. When experimental data are consistent within the expected error limits, s_{w} should be close to unity. In addition, use of the following statistical criteria was made: the *standard deviation*

$$s = \left(\frac{\Sigma_{i=1}^{n}(C_{\text{sm}} - C_{\text{exp}})_i^2}{n - m}\right)^{1/2}, \tag{8}$$

the *percentage standard deviation*

$$s_{\text{r}} = \left(\frac{\Sigma_{i=1}^{n}[(C_{\text{sm}} - C_{\text{exp}})/C_{\text{exp}}]_i^2}{n - m}\right)^{1/2} 100, \tag{9}$$

the *bias*

$$s_{\text{b}} = \frac{\Sigma_{i=1}^{n}(C_{\text{sm}} - C_{\text{exp}})_i}{n}, \tag{10}$$

and the difference between the number of experimental points with positive and negative deviations from the smoothed values (denoted in tables as +/−).

In order to get information on how data from individual sources compare with the final correlation, the deviations d_{w}, d, d_{r}, and d_{b} defined analogously to s_{w}, s, s_{r}, and s_{b} were calculated for both included and rejected data sets.

The definitions are as follows: the *average weighted deviation*

$$d_{\text{w}} = \left(\frac{\Sigma_{i=1}^{n_1}[(C_{\text{sm}} - C_{\text{exp}})^2/\sigma^2 C]_i}{n_1}\right)^{1/2}, \tag{11}$$

the *average deviation*

$$d = \left(\frac{\Sigma_{i=1}^{n_1}(C_{\text{sm}} - C_{\text{exp}})_i^2}{n_1}\right)^{1/2}, \tag{12}$$

the *average percentage deviation*

$$d_{\text{r}} = \left(\frac{\Sigma_{i=1}^{n_1}[(C_{\text{sm}} - C_{\text{exp}})/C_{\text{exp}}]_i^2}{n_1}\right)^{1/2} 100, \tag{13}$$

and the *bias* of a data set

$$d_b = \frac{\sum_{i=1}^{n_1}(C_{sm} - C_{exp})_i}{n_1}, \quad (14)$$

where n_1 denotes the number of data points in one data set.

When heat capacity was measured at one temperature only and several literature sources were available, simple selection of the best value or averaging of several measurements was performed.

3.3. Temperature correlation and establishment of recommended values

Two different approaches were adopted for correlating heat capacities as a function of temperature. *Polynomials or cubic spline polynomials* were used for accurately fitting heat capacity inside the temperature limits of experimental values. A *quasipolynomial equation* was also used when it was appropriate (see below); this equation enabled one to describe the temperature dependence by one set of parameters which, unlike polynomial equations, allows a meaningful extrapolation above the upper temperature limit of the experimental data.

3.3.1. Representation of data by polynomials

When data are available only in a limited temperature range, one polynomial of third or lower order may be sufficient for fitting the data successfully. In all cases, when such a condition was probable, the correlation with one polynomial was tried first. Its order was gradually increased to 3, and the statistical F test was used to determine when the addition of higher terms was not significant any longer.

Fitting with cubic splines was used only when the F test indicated need for a higher than third order polynomial. We used the correlation algorithm developed at the Technical University of Budapest (1979KOL) in which the two boundary conditions are considered during minimization as two additional adjustable parameters. Usually three and sometimes four knots were necessary for the satisfactory fit of the data within the expected experimental error limits.

The results of spline correlation are usually reported in terms of the knot values and two boundary conditions; the spline routine is then necessary for generating the recommended data. Since such a routine is not available to all users of the data, we preferred to tabulate directly the parameters of the cubic polynomials which are easier to use. This presentation is also consistent with the tabulation when only one polynomial is used. The tabulated adjustable parameters, A_j, relate to the equation expressing the dimensionless quantity C/R as a function of the scaled temperature $T/100$:

$$\frac{C}{\mathrm{R}} = \sum_{j=0}^{m} A_{j+1}\left(\frac{T}{100}\right)^j, \quad (15)$$

where R is the gas constant ($\mathrm{R} = 8.314\,472\ \mathrm{J\ K^{-1}\ mol^{-1}}$, see 2005MOH/TAY); scaling was made to improve the numerical stability of the fitting procedure. The upper limit of the summation m is equal to 3 in all cases where the overall temperature range is subdivided (cubic spline fitting) or can be lower when only one polynomial is used to describe the data.

3.3.2. Representation of data by a quasipolynomial equation

The quasipolynomial equation was used in the form derived by Zábranský *et al.* (1996ZAB/RUZ):

$$\frac{C}{\mathrm{R}} = A_1 \ln(1 - T_r) + \frac{A_2}{1 - T_r} + \sum_{j=0}^{m} A_{j+3} T_r^j, \quad (16)$$

where $T_r = T/T_c$, T_c is the critical temperature, and m equals 3 for about 50% of substances. The derivation of a quasipolynomial equation was based on the assumption that the heat capacity is always an increasing function of temperature and is unbounded at the critical point. The quasipolynomial equation was not used when fewer then seven experimental data points were available and the temperature range of experimental data was below 50 K or when there was no possibility of obtaining the critical temperature. In this work parameters of the quasipolynomial equation are not given if new experimental data do not extend over the upper temperature limit of the data presented in Monograph No. 6 (1996ZAB/RUZ) and/or Supplement I (2001ZAB/RUZ).

The variation of heat capacity in the high-temperature range differs considerably from one compound to another. It should be kept in mind that the quasipolynomial equation is mainly empirical and extrapolation above the upper temperature limit of experimental data is correct only in a qualitative manner. No guarantee can be given that the extrapolation will describe quantitatively the real heat capacity in this region except for the value at the critical point which is always correct and corresponds to plus infinity.

For organic substances, the critical temperatures from the data bank of the Institute of Chemical Technology, Prague (2000CDA) or from the TRC tables (2007FRE/HON) were used; for substances where T_c values were not found, estimates were performed according to Lydersen (1955LYD).

3.3.3. Types of heat capacities presented

When establishing the recommended values no distinction was made between the saturation heat capacity C_{sat} and the isobaric heat capacity C_p when their difference was smaller than the expected error of experimental data over the whole temperature range of their validity. This was the case for practically all substances where data did not reach above the normal boiling temperature. Then only one set of parameters was presented for each of the correlation equations.

For the compounds where experimental values of reasonable accuracy are available above the normal boiling temperature, distinct recommended data sets are presented for C_p and C_{sat}. In this case, all raw data were first converted to one type of heat capacity which was used in the evaluation and selection process. After the experimental values for the final correlation had been set, they were expressed as C_p and C_{sat}

and both sets were correlated separately under identical conditions using the polynomial or cubic spline representation. Only isobaric heat capacity C_p was correlated by the quasi-polynomial equation.

Recommended C_{sat} data relate by definition to the saturation line. Recommended C_p data relate above the normal boiling temperature to the saturation line. Below T_b, they represent both the heat capacity at standard pressure of 101.325 kPa and the saturation pressure as their difference is smaller than the accuracy of the best literature data.

When necessary, conversion between C_p and C_{sat} was performed using Eq. (4). As there are not enough data on expansivities, the term $(\partial V/\partial T)_p$ was approximated by $(\partial V/\partial T)_{sat}$; the difference between them becomes important only far above the normal boiling temperature. The latter term was calculated from the temperature correlation of densities along the saturation line using a modified Rackett equation (1985CAM/THO) or the Francis equation (1986SMI/SRI). The derivative, $(dp/dT)_{sat}$, was calculated from one of the following vapor pressure equations: Wagner, Frost-Kalkwarf, Cox, or Antoine using parameters from the references 1979DYK/REP, 1983MCG, 1984DYK/REP, and 1990CHI/GAM, respectively.

4. Guide to tables

4.1. Division of substances into groups

To make the data presentation logical and easy to follow, the compounds are divided into *sections* according to the kinds of atoms they contain. These are further divided into *groups* according to their chemical structure. This arrangement makes it possible to illustrate specific features of individual families of substances and to show the connection between the magnitude of the quantities listed and the chemical structure of individual substances. In this work we added a new important family of compounds, denoted as ionic liquids. The adopted ordering system can be seen in the following table. Each group is assigned a designated double digit. This organization is shown in Table 4.

TABLE 4. Division of compounds into groups

Main Group No.	Subgroup No.	Group name
0		**Inorganic Compounds**
	01	Elements
	02	Inorganic compounds
1		**Compounds of Carbon and Hydrogen**
	11	Saturated aliphatic hydrocarbons
	12	Saturated cyclic hydrocarbons
	13	Unsaturated aliphatic hydrocarbons
	14	Aromatic and unsaturated cyclic hydrocarbons
2		**Compounds of Carbon, Hydrogen, and Halogen**
	21	Fluorine derivatives
	22	Chlorine derivatives
	23	Bromine derivatives
	24	Iodine derivatives
	25	Mixed halogen derivatives
3		**Compounds of Carbon, Hydrogen, and Nitrogen**
	31	Amines
	32	Nitriles
	33	Heterocyclic nitrogen compounds
	34	Miscellaneous nitrogen compounds
4		**Compounds of Carbon, Hydrogen, and Oxygen**
	41	Ethers
	42	Alcohols and phenols
	43	Carbonyl compounds
	44	Acids and anhydrides
	45	Esters
	46	Heterocyclic oxygen compounds
	47	Miscellaneous oxygen compounds
5		**Compounds of Carbon, Hydrogen, and Sulfur**
	51	Sulfides
	52	Thiols
	53	Heterocyclic sulfur compounds
6		**Other Organic Compounds Containing Halogens, Nitrogen, Oxygen, and Sulfur**
	61	Compounds of carbon, hydrogen, halogen, and oxygen
	62	Compounds of carbon, hydrogen, nitrogen, and oxygen
	63	Compounds of carbon, hydrogen, oxygen, and sulfur
	64	Miscellaneous compounds
7		**Organic Compounds Containing Other Elements than Halogens, Nitrogen, Oxygen, and Sulfur**
	71	Organosilicon compounds
	72	Organic compounds containing phosphorus and boron
	73	Organometallic compounds
	74	Salts of organic acids
	75	Ionic liquids

The substances of section 0 (elements and inorganic compounds) are ordered according to their formulas in alphabetical order. Organic compounds (sections 1–7) are ordered within each group according to the usual convention (Hill system), i.e., in order of increasing number of carbon and hydrogen atoms. Other elements are placed in alphabetical order. The substances having the same molecular formula are arranged in alphabetical order according to their names. Two numbers separated by a dash, the so-called *group-member number*, code each substance. The first two-digit number indicates the group (family of substances), and the second three-digit number denotes the serial number of a substance inside the group. In naming the substances, we adopted the Chemical Abstracts rules for the names under which the sub-

stance was presented with the exception of simple esters where we used shorter names, e.g., methyl acetate instead of methyl ester acetic acid. Codes for individual substances permitting their location inside the tables and the corresponding CAS registry numbers can be found in the formula index at the end of the paper.

New compounds from Supplement II, not included in Monograph No. 6 and in Supplement I, were put in the appropriate group after the last compound covered by Monograph No. 6 and/or Supplement I and then listed according to the Hill system. This retains the numbering of all compounds from Monograph No. 6 and Supplement I and makes it possible to find a particular compound from the knowledge of its group-member number.

Several specific tags were appended to the group-member number to distinguish between compounds located in this work and in Supplement I (2001ZAB/RUZ). The specific tags are described in more detail in Sec. 5.

4.2. Tables and deviation plots

Most of the information on the data and their processing is given for each substance in tables which are described in detail below. Methodology and procedure which led to this presentation of data are described in Sec. 3. The tables for each substance are preceded with name of the substance, its formula, group-member number, and CAS registry number.

The characterization of raw data, their consistency, and results of correlation and recommended data are summarized for each substance separately in three to four tables and a deviation plot.

A table of *experimental heat capacities* (table type number 1) reviews all primary sources and characterizes briefly experimental conditions and the quality of data. For those compounds where new experimental data published after 2000 do not improve the uncertainty of recommended data and/or do not extend the temperature range only this table is presented in this paper.

The upper half of the table of *correlated heat capacities* (table type number 2) lists sources selected for establishing the recommended values; the statistical criteria defined by Eqs. (8)–(15) indicate for both selected and discarded sources how the individual data sets compare with values generated from the correlation equation. The consistency of raw data is graphically demonstrated in the *deviation plot*. The table of correlated heat capacities is not present when the data are available at only one temperature or when there is only one literature source.

The table listing *parameters of polynomial(s)* (table type number 3) obtained by fitting the selected data also gives information on the quality of the overall fit and reliability of the recommended data.

Parameters of quasipolynomial equation (table type number 4) are presented for substances where application of this relationship is meaningful.

Each table is coded with three numbers separated by periods. The first two numbers are identical with the substance code (see Sec. 4.1) and the third relates to the type of table (1–4). Even when some tables are missing, the numbering related to the type of table is retained.

The symbol C without a subscript specification or the term heat capacity are used in tables whenever we refer both to C_p and C_{sat} at temperatures where the difference between their values is negligible compared with the expected experimental error.

Certain statistics and parameters are listed in the modified E notation. The first part of the number denotes the fractional part which is followed by the exponent to the base 10. The exponent is separated from the fractional part by a plus or a minus sign (e.g., $-1.53-5$ means -1.53×10^{-5}).

4.2.1. Experimental heat capacities

Each line of the table contains information on one literature source of experimental data. When several distinct data sets were given for the same substance in one publication (for example, parameters of smoothing equations relating to different temperature subintervals or the data obtained from two different calorimeters) there are several lines for one data source, each relating to one data set.

***First column*. Reference [Note]:** The abbreviated reference in the form YYYYAAA/BBBM where YYYY is the year of publication, AAA and BBB are the first three letters of the last name of the first and second authors (if present), respectively. M is a digit from 1 to 9 distinguishing papers published by the same author(s) within the same year. If the same data set appeared in two or more different publications the reference to the earliest source is given; an appropriate note is given below the table. For some sources, a footnote is added below the table. In these cases, there is a capital N between the first and second columns.

***Second column. T*/K**: Temperature range of the data set in kelvins.

***Third column.* nPts:** Number of experimental data points; the symbol "eqn" is used in those cases where only parameters of a smoothing equation were presented in the original literature; the symbol "S" denotes that the discrete values given in the original literature source were generated from a smoothing equation.

***Fourth column.* Err/%:** Error of measurement, $\sigma_r C_{\mathrm{exp}}$, in percentage claimed by the author(s); the abbreviation "n/a" (not available) is used when no specification is given in the original literature.

***Fifth column.* Pur/% [Method]:** Purity of the substance in percentage (given with the same number of significant digits as in the original source) and analytical method used for its determination; the meaning of the abbreviations used is as follows: "anal," analytical (used when the analytical method was not specified); "chrom," gas or liquid chromatography; "estim," the purity was estimated by the author(s); "melpt," determination of impurities from the melting point depression.

***Sixth column.* Type:** Type of heat capacity reported in the original literature; p, isobaric heat capacity, sat, saturation

heat capacity, avg, average heat capacity determined over a temperature range usually greater than 10 K.

Seventh column. **Calor [Cal Reference]:** Calorimetric method used for determining the data and reference to the publication where the instrument is described. The coding used for classification of experimental techniques is introduced in Table 1 and the individual types of calorimeters are summarized in Table 2. The criteria for classifying heat capacity calorimeters are discussed in Sec. 2. All references to calorimeters listed in tables of experimental heat capacities are summarized in Table 3.

4.2.2. Correlated heat capacities

This table contains information on the results of the correlation presented for the individual data sets. The statistics for the selected and rejected data sets are listed in the upper and lower halves of the table, respectively. The meaning of the columns in the *upper part* of the table is as follows.

First column. **Reference:** The abbreviated reference (the same as in the table of experimental heat capacities).

Second column. $T/\mathbf{K}$: Temperature range (K) in which the data from a particular source were included in the correlation.

Third column. **nPts:** Number of values used in the final determination of the correlation parameters. The entries in the second and third columns are identical to those in the table of experimental heat capacities when the whole data set was included in the correlation; they differ if part of the data was discarded.

Fourth column. $\sigma_r C/\%$: Percentage error used in Eq. (6) to estimate the variance of individual data points. This value is either $\sigma_r C_{exp}$ (column 4 in the table of experimental heat capacities) or is assigned by the evaluator in cases when no error is specified in the original source or the author's estimate does not seem to be realistic. When $\sigma_r C$ was assigned or modified by the evaluator, the value is followed by the sign #.

Fifth column. d_w: Average weighted deviation defined by Eq. (11).

Sixth column. $d/\mathbf{R}$: Average deviation, defined by Eq. (12) divided by R (dimensionless).

Seventh column. d_r: Average percentage deviation, defined by Eq. (13).

Eighth column. $d_b/\mathbf{R}$: Bias of the data set, defined by Eq. (14), divided by R (dimensionless).

Ninth column. **+/−:** The difference between the number of experimental points with positive and negative deviations from the recommended values.

In the *lower part* of the table, the quantities $d/\mathbf{R}$, d_r, d_b/R, and +/− are presented in parenthesis for each reference rejected from the final correlation. Information is not given for rejected data sets when they fall outside of the selected temperature range.

In some cases, the correlations for isobaric and saturation heat capacities were performed separately. We give, however, only one table of correlated heat capacities for these compounds as the selection of data sources did not differ and statistical values were practically identical in both correlations.

4.2.3. Parameters of polynomials

This table contains parameters for both isobaric and saturation heat capacities when these two quantities can be distinguished or it contains parameters referring to the type of heat capacity given in the table of experimental heat capacities. The symbol C is used when referring to both C_p and C_{sat}.

The table gives characteristics of the final correlation of the selected data in the upper part and the corresponding parameters of the polynomial(s) in the lower part.

The *upper part* consists of two lines when both isobaric and saturation heat capacities are tabulated and of only one line when no distinction is made between the two heat capacities. The following items are listed.

First column. **Type:** Type of heat capacity listed—*p* and sat denote isobaric and saturation heat capacities, respectively. The *C* is used when no distinction was made between the two types of heat capacities.

Second column. **nTot:** The total number of all experimental data points available.

Third column. **nPts:** The total number of experimental data points used in the correlation.

Fourth column. s_w: The standard weighted deviation, defined by Eq. (7).

Fifth column. $s/\mathbf{R}$: Standard deviation, defined by Eq. (8), divided by R (dimensionless).

Sixth column. s_r: Standard percentage deviation, defined by Eq. (9).

Seventh column. s_b: Bias, defined by Eq. (10), divided by R (dimensionless).

Eighth column. **+/−:** The overall difference between the numbers of experimental points with positive and negative deviations from the recommended values.

The parameters of the cubic spline polynomials describing individual subintervals of the temperature range of the selected data are listed in the *lower part* of the table. When the isobaric and saturation heat capacities are distinguished, two sets of parameters are listed separately, the first set relating to the temperature correlation of C_p and the second to that of C_{sat}. When the whole temperature range of experimental data is described by only one equation the parameters were obtained by simple unconstrained fitting using a polynomial of third or lower degree. The meaning of the individual columns is as follows:

First column: Temperature subinterval in kelvins to which the listed parameters relate.

Second to fifth columns: Parameters of the polynomial defined by Eq. (15) valid in the given subinterval. Dimension of the parameters is T^{-j}.

Sixth column: Level of uncertainty assigned by the evaluators to the data generated from the polynomial in the given temperature subinterval. This characteristic expresses the ex-

pected overall uncertainty of the recommended data and reflects both the uncertainty in the experimental values and possible error due to the fitting procedure. The following levels of uncertainty were assigned: I, excellent data (uncertainty below 0.1%); II, highly reliable data (uncertainty below 0.3%); III, reliable data (uncertainty below 0.5%); IV, medium quality data (uncertainty below 1%); V, data of low reliability (uncertainty below 3%); VI, very unreliable data with a possibility of gross systematic errors (uncertainty above 3%).

The level of uncertainty assigned to individual subintervals for cubic splines often differs due to the unequal reliability of experimental data in different parts of the temperature range. On the other hand in certain cases one set of parameters was used for describing two (or exceptionally three) experimental data sets of different accuracies, which related to different temperature ranges. Then the level of uncertainty assigned to recommended data relates always to the data set of lower quality; in reality the recommended data are more reliable than indicated at temperatures where the experimental data set of higher quality was available. The reader can obtain information regarding changes in reliability within the temperature interval of recommended data from the table of correlated heat capacities.

4.2.4. Parameters of the quasipolynomial equation

The quasipolynomial equation (16) is useful as a simple expression permitting extrapolations to higher temperatures. The quasipolynomial fit was performed only for isobaric heat capacity as the application of this quantity is wider compared to C_{sat}. In all other cases where C_p and C_{sat} heat capacities are identical within error of measurement parameters of the quasipolynomial equation are presented for a single type of the heat capacity presented in the table.

The table is organized analogously to the table presenting parameters of polynomials; the *upper part* of the table is identical. The items tabulated in the *lower part* have the following meaning.

First column. T/K: Temperature interval (K) to which the listed parameters relate. This interval is not necessarily identical with the temperature range of the representation by polynomials.

Second column. T_c/K: Critical temperature (K).

Third to eighth columns. A_1, A_2, A_3, A_4, A_5, A_6: Four or six parameters of the quasipolynomial equation ($m=1$ or 3). The parameters are dimensionless.

Ninth column. **Uncert:** Level of uncertainty assigned by the evaluators to the data generated from the quasipolynomial equation within the temperature range of the experimental data. When using the equation outside this range, the uncertainty decreases with the length of the extrapolation.

4.2.5. Deviations plots

An overview of the deviations from the recommended values for all experimental data (both included in and rejected from the final correlation) measured by various authors is presented in graphical form in the deviation plots. The temperature is plotted along the x axis and the relative percentage deviation for individual data points along the y axis. Data from different sources are distinguished by different symbols. Points that lie outside the range of the ordinate in the plot are accompanied by the numerical value of the deviation. Some points that overlap each other or the accompanying figures are omitted. When too many data points were available, some less important sets and values exhibiting large deviations from the recommended data were not included. The abbreviated references below the deviation plot are given in the form YYAAA/BBBM where YY is the last two digits of the year of publication (for a year before 1900 the reference code is preceded by an asterisk, *, and for the year 2000 and after the reference code is preceded by a pound sign, #), AAA, BBB, and M have the same meaning as explained in Sec. 4.2.1.

5. Formula index of compounds

The formula index of compounds given in Table 5 lists all compounds for which data were compiled and presented in Monograph No. 6 (1996ZAB/RUZ) and Supplement I (2001ZAB/RUZ) and includes also newly compiled data. This enables the reader to locate data for a particular compound.

Compounds are sorted in the order of empirical formulas. The empirical formula is given in the first column. The second column gives the Chemical Abstracts Service Registry Number (CAS RN). The third column lists the group-member number. The system of dividing compounds into groups is described in detail in Sec. 4.1. The first two-digit number indicates the group, and the second three-digit number denotes the serial number of a compound inside the group. Tables in the compilation are coded with three numbers separated by full stops. The first two numbers are identical with the compound group and member number. The fourth and fifth columns give the name of a compound and, if present, synonyms, common names, or commercial names.

If there are more compounds with the same empirical formula, they are listed under a common formula.

For geometric isomers which are common among alkenes the symbols (*Z*) and (*E*) are used to identify the stereochemistry of groups of highest priority either on the same side of the double bond or across from the double bond. For simple systems (*Z*) and (*E*) are equivalent to *cis* and *trans*.

Several specific tags were appended to the group-member number to distinguish between compounds located in this work, in Monograph No. 6, and in Supplement I or in any combination of all works. The tag is separated from the group-member number by a slash. No tag means the compound is present in Monograph No. 6 only. The tag /S1 denotes compounds present in Supplement I (2001ZAB/RUZ) only, the tag /B+S1 denotes compounds present both in Monograph No. 6 and in Supplement I, the tag /B+S2 denotes compounds present both in Monograph No. 6 and in this work with a new set of correlation equation parameters

given in this work, the tag /S1+S2 denotes compounds present in both supplements, and the tag /B+S1+S2 denotes compounds present in Monograph and in both supplements.

TABLE 5. Formula index of compounds

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$AgNO_3$	7761-88-8	02-001 /B+S2	Silver(1+) salt nitric acid	Silver nitrate
$AlBr_3$	7727-15-3	02-002	Aluminum bromide	
$AlCl_3$	7446-70-0	02-003	Aluminum chloride	
AlI_3	7784-23-8	02-004	Aluminum iodide	
Ar	7440-37-1	01-001	Argon	
$AsCl_3$	7784-34-1	02-005	Arsenous trichloride	Arsenic trichloride; Arsenic chloride
AsF_3	7784-35-2	02-006	Arsenous trifluoride	Arsenic trifluoride
AsH_3	7784-42-1	02-007	Arsine	
BF_3	7637-07-2	02-008 /B+S1	Trifluoroborane	Boron fluoride (BF_3); Boron trifluoride
B_2Cl_4	13701-67-2	02-009	Boron chloride (B_2Cl_4)	Diboron tetrachloride
B_2H_6	19287-45-7	02-010	Diborane	
$B_3H_6N_3$	6569-51-3	02-011	Borazine	Borazole
B_5H_9	19624-22-7	02-012	Pentaborane	
$B_{10}H_{14}$	17702-41-9	02-013	Decaborane	
Bi	7440-69-9	01-002	Bismuth	
BrD	13536-59-9	02-014	Hydrobromic acid-*d*	Deuterium bromide
BrF_3	7787-71-5	02-015	Bromine fluoride (BrF_3)	Bromine trifluoride
BrH	10035-10-6	02-016	Hydrobromic acid	Hydrogen bromide
BrIn	14280-53-6	02-017	Indium bromide (InBr)	
Br_2	7726-95-6	01-003	Bromine	
Br_2Sn	10031-24-0	02-018	Tin bromide ($SnBr_2$)	
Br_4Sn	7789-67-5	02-019	Tetrabromostannane	Tin(IV) bromide; Tin tetrabromide
$CBrCl_3$	75-62-7	25-001	Bromotrichloromethane	
$CBrF_3$	75-63-8	25-002	Bromotrifluoromethane	R13B1
CBr_4	558-13-4	23-001	Tetrabromomethane	Carbon tetrabromide; Perbromomethane
$CClF_3$	75-72-9	25-003	Chlorotrifluoromethane	R13
$CClN_3O_6$	1943-16-4	64-001	Chlorotrinitromethane	
CCl_2F_2	75-71-8	25-004 /B+S1	Dichlorodifluoromethane	R12
CCl_2O	75-44-5	02-020	Carbonic dichloride	Phosgene
CCl_3F	75-69-4	25-005	Trichlorofluoromethane	R11
CCl_4	56-23-5	22-001 /B+S1	Tetrachloromethane	Carbon tetrachloride; Perchloromethane
CD_4	558-20-3	11-001	Methane-d_4	Deuteromethane
CD_4O	811-98-3	42-106 /S1	Methanol-d_4	Methyl-d_3 alcohol-*d*
CF_2O	353-50-4	02-021	Carbonic difluoride	Carbonyl fluoride
CF_4	75-73-0	21-001 /B+S1	Tetrafluoromethane	Carbon tetrafluoride; Perfluoromethane; R14
$CHBr_3$	75-25-2	23-002	Tribromomethane	Bromoform; Methenyl tribromide
$CHClF_2$	75-45-6	25-006	Chlorodifluoromethane	R22
$CHCl_2F$	75-43-4	25-007	Dichlorofluoromethane	R21
$CHCl_3$	67-66-3	22-002 /B+S1	Trichloromethane	Chloroform; Methenyl trichloride
CHD_3O	1849-29-2	42-107 /S1	Methan-d_3-ol	Methyl-d_3 alcohol
CHF_3	75-46-7	21-002 /B+S2	Trifluoromethane	Fluoroform; R23
CHF_3S	1493-15-8	64-002	Trifluoromethanethiol	
$CHLiO_2$	556-63-8	74-023 /S1	Lithium salt formic acid	Lithium formate; Lithium methanoate

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
CHN	74-90-8	02-022	Hydrocyanic acid	Hydrogen cyanide
$CHNaO_2$	141-53-7	74-001	Sodium salt formic acid	Sodium formate; Natrium formate
CH_2Br_2	74-95-3	23-003 /B+S1	Dibromomethane	Methylene bromide
CH_2Cl_2	75-09-2	22-003	Dichloromethane	Methylene chloride
CH_2F_2	75-10-5	21-034 /S1	Difluoromethane	Methylene difluoride; R32
CH_2I_2	75-11-6	24-001 /B+S1	Diiodomethane	Methylene iodide
CH_2N_2	420-04-2	34-001	Cyanamide	
CH_2O_2	64-18-6	44-001 /B+S1	Formic acid	Methanoic acid; Hydrogen carboxylic acid
CH_2S_3	594-08-1	02-023	Trithiocarbonic acid	Dihydrosulfide carbon sulfide
CH_3Br	74-83-9	23-004	Bromomethane	Methyl bromide
CH_3Cl	74-87-3	22-004	Chloromethane	Methyl chloride
CH_3ClFOP	753-71-9	72-001	Methylphosphonic chloride fluoride	Methylphosphonic chlorofluoride
CH_3Cl_2OP	676-97-1	72-002	Methylphosphonic dichloride	
CH_3Cl_3Si	75-79-6	71-057 /S1	Trichloromethylsilane	
CH_3D	676-49-3	11-002	Methane-*d*	Monodeuteromethane
CH_3DO	1455-13-6	42-001 /B+S1	Methanol-*d*	Monodeuteromethanol
CH_3F_2OP	676-99-3	72-003	Methylphosphonic difluoride	
CH_3I	74-88-4	24-002 /B+S1	Iodomethane	Methyl iodide
CH_3NO	75-12-7	62-001 /B+S1	Formamide	Methanamide
CH_3NO_2	75-52-5	62-002 /B+S1+S2	Nitromethane	
CH_3NO_3	598-58-3	62-003	Methyl ester nitric acid	Methyl nitrate
CH_4	74-82-8	11-003	Methane	
CH_4N_2O	57-13-6	62-004	Urea	Carbamide
CH_4O	67-56-1	42-002 /B+S1+S2	Methanol	Methyl alcohol; Carbinol; Wood alcohol
CH_4S	74-93-1	52-001	Methanethiol	Methyl mercaptan
CH_5N	74-89-5	31-001	Methanamine	Methylamine; Aminomethane
CH_6N_2	60-34-4	34-002	Methylhydrazine	Monomethylhydrazine
CO	630-08-0	02-024	Carbon monoxide	
COS	463-58-1	02-025	Carbon oxide sulfide	Carbonyl sulfide
CO_2	124-38-9	02-026 /B+S1	Carbon dioxide	
CS_2	75-15-0	02-027	Carbon disulfide	
CSe_2	506-80-9	02-028	Carbon selenide (CSe_2)	
$C_2Br_2D_4$	22581-63-1	23-005	1,2-Dibromoethane-1,1,2,2-d_4	1,2-Dibromodeuteroethane
$C_2Br_2F_4$	124-73-2	25-008	1,2-Dibromo-1,1,2,2-tetrafluoroethane	R114B2
$C_2Br_3D_3$		23-006	1,1,2-Tribromoethane-1,2,2-d_3	
C_2ClF_3	79-38-9	25-009	Chlorotrifluoroethene	Chlorotrifluoroethylene
C_2ClF_5	76-15-3	25-010	Chloropentafluoroethane	R115
$C_2Cl_2F_4$	76-14-2	25-012 /B+S1	1,2-Dichloro-1,1,2,2-tetrafluoroethane	*sym*-Dichlorotetrafluoroethane;Fluorocarbon-114; R114
	1320-37-2	25-011	Dichlorotetrafluoroethane (unspecified isomer)	
$C_2Cl_3F_3$	354-58-5	25-013	1,1,1-Trichloro-2,2,2-trifluoroethane	
	76-13-1	25-014	1,1,2-Trichloro-1,2,2-trifluoroethane	R113
C_2Cl_4	127-18-4	22-005 /B+S2	Tetrachloroethene	Perchloroethylene
$C_2Cl_4F_2$	76-12-0	25-015	1,1,2,2-Tetrachloro-1,2-difluoroethane	*sym*-Tetrachlorodifluoroethane; R112
$C_2F_2O_2$	359-40-0	61-001	Ethanedioyl difluoride	Oxalyl fluoride
C_2F_3N	353-85-5	64-003	Trifluoroacetonitrile	Trifluoroethanenitrile; Trifluoromethyl cyanide
C_2F_4	116-14-3	21-003	Tetrafluoroethene	Perfluoroethylene
C_2F_4O	354-34-7	61-002	Trifluoroacetyl fluoride	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
C_2F_6	76-16-4	21-004	Hexafluoroethane	Perfluoroethane
$C_2HBrClF_3$	354-06-3	25-016	1-Bromo-2-chloro-1,1,2-trifluoroethane	
	151-67-7	25-017	2-Bromo-2-chloro-1,1,1-trifluoroethane	Halothane
$C_2HBr_2D_3$	117164-17-7	23-007	1,2-Dibromoethane-1,1,2-d_3	
$C_2HBr_3D_2$		23-008	1,1,2-Tribromoethane-2,2-d_2	
C_2HClF_4	2837-89-0	25-036 /S1+S2	2-Chloro-1,1,1,2-tetrafluoroethane	Monochloro-1,1,1,2-tetrafluoroethane; R124
$C_2HCl_2F_3$	354-23-4	25-037 /S1	1,2-Dichloro-1,1,2-trifluoroethane	R123a
	306-83-2	25-038 /S1+S2	2,2-Dichloro-1,1,1-trifluoroethane	R123
C_2HCl_3	79-01-6	22-006	Trichloroethene	Trichloroethylene
$C_2HCl_3F_2$	354-15-4	25-018	1,1,2-Trichloro-1,2-difluoroethane	R122
	354-21-2	25-039 /S1	1,2,2-Trichloro-1,1-difluoroethane	R122a
C_2HCl_3O	75-87-6	61-003 /B+S2	Trichloroacetaldehyde	Trichloroethanal; Chloral
$C_2HCl_3O_2$	76-03-9	61-004	Trichloroacetic acid	Trichloroethanoic acid
C_2HCl_5	76-01-7	22-007	Pentachloroethane	Pentalin
C_2HF_5	354-33-6	21-035 /S1	Pentafluoroethane	R125
C_2HF_5O	3822-68-2	61-047 /S1	(Difluoromethoxy)trifluoromethane	Difluoromethyl trifluoromethyl ether
C_2H_2	74-86-2	13-039 /S1	Ethyne	Acetylene
$C_2H_2AsCl_3$	50361-05-2	73-033 /S1	(*E*)-(2-Chloroethenyl)arsonous dichloride	*trans*-Chlorovinyldichlorarsine; *β*-Chlorovinyldichlorarsine; *β*-Lewisite
$C_2H_2Br_2D_2$		23-009	1,2-Dibromoethane-1,1-d_2	
		23-010	1,2-Dibromoethane-1,2-d_2	
$C_2H_2Br_3D$		23-011	1,1,2-Tribromoethane-1-d_1	
		23-012	1,1,2-Tribromoethane-2-d_1	
$C_2H_2Br_4$	79-27-6	23-013	1,1,2,2-Tetrabromoethane	*sym*-Tetrabromoethane; Acetylene tetrabromide
$C_2H_2Cl_2$	75-35-4	22-008	1,1-Dichloroethene	1,1-Dichloroethylene; Vinylidene chloride
	540-59-0	22-009	1,2-Dichloroethene	1,2-Dichloroethylene (unspec. isomer)
	156-60-5	22-010	(*E*)-1,2-Dichloroethene	*trans*-1,2-Dichloroethene; *trans*-1,2-Dichloroethylene
	156-59-2	22-011	(*Z*)-1,2-Dichloroethene	*cis*-1,2-Dichloroethene; *cis*-1,2-Dichloroethylene
$C_2H_2Cl_2F_2$	1842-05-3	25-019	1,1-Dichloro-1,2-difluoroethane	R132
$C_2H_2Cl_2O_2$	79-43-6	61-005	Dichloroacetic acid	Dichloroethanoic acid
$C_2H_2Cl_4$	630-20-6	22-012	1,1,1,2-Tetrachloroethane	
	79-34-5	22-013	1,1,2,2-Tetrachloroethane	*sym*-Tetrachloroethane; Acetylene tetrachloride
$C_2H_2F_3NO$	354-38-1	64-031 /S1	2,2,2-Trifluoroacetamide	
$C_2H_2F_4$	811-97-2	21-036 /S1	1,1,1,2-Tetrafluoroethane	R134a
C_2H_3Br	593-60-2	23-014	Bromoethene	Bromoethylene; Vinyl bromide
$C_2H_3Br_2D$		23-015	1,2-Dibromoethane-d_1	
$C_2H_3Br_3$	78-74-0	23-016	1,1,2-Tribromoethane	
C_2H_3Cl	75-01-4	22-014	Chloroethene	Vinyl chloride
$C_2H_3ClF_2$	75-68-3	25-020	1-Chloro-1,1-difluoroethane	R142
C_2H_3ClO	75-36-5	61-006	Acetyl chloride	Ethanoyl chloride
$C_2H_3ClO_2$	79-11-8	61-007	Chloroacetic acid	Chloroethanoic acid
$C_2H_3Cl_2F$	1717-00-6	25-040 /S1	1,1-Dichloro-1-fluoroethane	R141b
$C_2H_3Cl_3$	71-55-6	22-015	1,1,1-Trichloroethane	Methylchloroform
	79-00-5	22-016	1,1,2-Trichloroethane	Vinyl trichloride; *β*-Trichloroethane
$C_2H_3Cl_3Si$	75-94-5	71-001	Trichloroethenylsilane	Trichlorovinylsilane
$C_2H_3F_3$	420-46-2	21-005	1,1,1-Trifluoroethane	
$C_2H_3F_3O$	75-89-8	61-008	2,2,2-Trifluoroethanol	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_2H_3LiO_2$	546-89-4	74-024 /S1	Lithium salt acetic acid	Lithium acetate; Lithium ethanoate
C_2H_3N	75-05-8	32-002	Acetonitrile	Ethanenitrile
C_2H_4	74-85-1	13-001	Ethene	Ethylene
C_2H_4BrCl	107-04-0	25-021	1-Bromo-2-chloroethane	Ethylene chlorobromide
C_2H_4Br2	106-93-4	23-017 /B+S1+S2	1,2-Dibromoethane	Ethylene dibromide
$C_2H_4Cl_2$	75-34-3	22-017	1,1-Dichloroethane	Ethylidene chloride
	107-06-2	22-018 /B+S1+S2	1,2-Dichloroethane	Ethylene dichloride
$C_2H_4D_2O_2$	2219-52-5	42-003	1,2-Ethanediol-d_2	Dideutero-1,2-ethanediol; Dideuteroethylene glycol
$C_2H_4F_2$	75-37-6	21-037 /S1	1,1-Difluoroethane	R152a
$C_2H_4N_4$	461-58-5	34-014 /S1	Cyanoguanidine	Dicyandiamide
C_2H_4O	75-07-0	43-001	Acetaldehyde	Ethanal
	75-21-8	46-001	Oxirane	Epoxyethane; Ethylene oxide
$C_2H_4O_2$	64-19-7	44-002 /B+S1+S2	Acetic acid	Ethanoic acid; Methane carboxylic acid; Vinegar acid
	107-31-3	45-001	Methyl formate	Methyl methanoate
C_2H_5Br	74-96-4	23-018 /B+S1+S2	Bromoethane	Ethyl bromide
C_2H_5Cl	75-00-3	22-019	Chloroethane	Ethyl chloride
$C_2H_5Cl_3Si$	115-21-9	71-002	Trichloroethylsilane	
C_2H_5DO	925-93-9	42-004	Ethanol-*d*	Monodeuteroethanol
C_2H_5I	75-03-6	24-003 /B+S1	Iodoethane	Ethyl iodide
C_2H_5N	151-56-4	33-001	Aziridine	Ethyleneimine
C_2H_5 NO	60-35-5	62-005 /B+S1	Acetamide	Ethanamide
	123-39-7	62-006	*N*-Methylformamide	
$C_2H_5NO_2$	79-24-3	62-007	Nitroethane	
$C_2H_5NO_3$	625-58-1	62-008	Ethyl nitrate	Ethyl ester nitric acid
C_2H_6	74-84-0	11-004 /B+S1	Ethane	
C_2H_6Cd	506-82-1	73-001	Dimethylcadmium	
$C_2H_6Cl_2Si$	75-78-5	71-058 /S1	Dichlorodimethylsilane	
	1789-58-8	71-003	Dichloroethylsilane	
C_2H_6O	64-17-5	42-005 /B+S1+S2	Ethanol	Ethyl alcohol; Grain alcohol
	115-10-6	41-001	Oxybis(methane)	Dimethyl ether; Methyl ether; Methyl oxide; Wood ether
C_2H_6OS	67-68-5	63-001 /B+S1+S2	Sulfinylbis(methane)	Dimethyl sulfoxide; DMSO
$C_2H_6O_2$	107-21-1	42-006 /B+S1+S2	1,2-Ethanediol	Ethylene glycol; Glycol
$C_2H_6O_2S$	67-71-0	63-002	Sulfonylbis(methane)	Dimethyl sulfone
C_2H_6S	75-08-1	52-002	Ethanethiol	Ethyl mercaptan
	75-18-3	51-001	Thiobis(methane)	Dimethyl sulfide
$C_2H_6S_2$	624-92-0	51-002	2,3-Dithiabutane	Dimethyl disulfide; Methyl disulfide
C_2H_6Se	593-79-3	73-002	Selenobis(methane)	Dimethyl selenide; Methyl selenide
$C_2H_6Se_2$	7101-31-7	73-003	Dimethyl diselenide	Methyl diselenide
C_2H_6Te	593-80-6	73-034 /S1	Tellurobis(methane)	Dimethyltellurium
C_2H_6Zn	544-97-8	73-004	Dimethylzinc	
C_2H_7N	75-04-7	31-002	Ethanamine	Ethylamine
	124-40-3	31-003	*N*-Methylmethanamine	Dimethylamine
C_2H_7NO	141-43-5	62-128 /S1	2-Aminoethanol	Ethanolamine
$C_2H_8N_2$	57-14-7	34-003	1,1-Dimethylhydrazine	*unsym*-Dimethylhydrazine
	540-73-8	34-004	1,2-Dimethylhydrazine	*sym*-Dimethylhydrazine

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	107-15-3	31-004 /B+S2	1,2-Ethanediamine	Ethylenediamine; 1,2-Diaminoethane
$C_2H_8N_2O_3$	22113-86-6	62-009	Nitrate ethylamine	Ethylammonium nitrate
$C_2H_{11}B_2N$	22580-01-4	72-004	(Dimethylamino)diborane	
C_2N_2	460-19-5	32-001	Ethanedinitrile	Cyanogen
C_3Cl_6	1888-71-7	22-050 /S1	1,1,2,3,3,3-Hexachloro-1-propene	Hexachloropropene; Hexachloropropylene
C_3F_6O	684-16-2	61-009	1,1,1,3,3,3-Hexafluoro-2-propanone	Hexafluoroacetone; Perfluoroacetone
C_3F_8	76-19-7	21-006	Octafluoropropane	Perfluoropropane
C_3HClF_6	359-58-0	25-041 /S1	1-Chloro-1,1,2,3,3,3-hexafluoropropane	R226ea
	431-87-8	25-042 /S1	2-Chloro-1,1,1,3,3,3-hexafluoropropane	R226da
$C_3HCl_2F_5$	431-86-7	25-043 /S1	1,2-Dichloro-1,1,3,3,3-pentafluoropropane	R225da
	422-48-0	25-044 /S1	2,3-Dichloro-1,1,1,2,3-pentafluoropropane	R225ba
C_3HF_7	2252-84-8	21-038 /S1	1,1,1,2,2,3,3-Heptafluoropropane	R227ca
	431-89-0	21-039 /S1	1,1,1,2,3,3,3-Heptafluoropropane	R227ea
$C3H_2ClF_5$	422-02-6	25-045 /S1	3-Chloro-1,1,1,2,2-pentafluoropropane	R235ca
$C_3H_2ClF_5$	460-92-4	25-022	1-Chloro-1,1,3,3,3-pentafluoropropane	
$C_3H_2Cl_2F_4$	146916-90-7	25-046 /S1	2,3-Dichloro-1,1,1,3-tetrafluoropropane	R234da
$C_3H_2Cl_2O_3$	3967-55-3	61-048 /S1	4,5-Dichloro-1,3-dioxolan-2-one	
$C_3H_2Cl_3F_3$	7125-84-0	25-023	1,1,1-Trichloro-3,3,3-trifluoropropane	
$C_3H_2F_6$	677-56-5	21-040 /S1	1,1,1,2,2,3-Hexafluoropropane	R236cb
	431-63-0	21-041 /S1	1,1,1,2,3,3-Hexafluoropropane	R236ea
	690-39-1	21-042 /S1	1,1,1,3,3,3-Hexafluoropropane	R236fa
$C_3H_2N_2$	109-77-3	32-003	Propanedinitrile	Malononitrile; Dicyanomethane
$C_3H_3ClO_3$	3967-54-2	61-049 /S1	4-Chloro-1,3-dioxolan-2-one	
$C_3H_3Cl_2F_3$	460-69-5	25-024	3,3-Dichloro-1,1,1-trifluoropropane	
$C_3H_3Cl_2F_3$	338-75-0	25-047 /S1	2,3-Dichloro-1,1,1-trifluoropropane	R243da
$C_3H_3Cl_3O_2$	598-99-2	61-010	Methyl trichloroacetate	Methyl ester trichloroacetic acid
$C_3H_3F_5$	1814-88-6	21-043 /S1	1,1,1,2,2-Pentafluoropropane	R245cb
	460-73-1	21-044 /S1	1,1,1,3,3-Pentafluoropropane	R245fa
	679-86-7	21-045 /S1	1,1,2,2,3-Pentafluoropropane	R245ca
C_3H_3N	107-13-1	32-004 /B+S1	2-Propenenitrile	Acrylonitrile; Vinyl cyanide
C_3H_3NO	288-14-2	62-010 /B+S1	Isoxazole	
	288-42-6	62-011	Oxazole	
C_3H_3NS	288-47-1	64-004	Thiazole	
$C_3H_3N_3$	290-87-9	33-002	1,3,5-Triazine	*sym*-Triazine
$C_3H_4ClF_3$	460-35-5	25-025	3-Chloro-1,1,1-trifluoropropane	
$C_3H_4Cl_2O_2$	116-54-1	61-011	Methyl dichloroacetate	Methyl ester dichloroacetic acid
$C_3H_4Cl_3NSi$	1071-22-3	71-004	3-Trichlorosilylpropanenitrile	
$C_3H_4Cl_4$	1070-78-6	22-020	1,1,1,3-Tetrachloropropane	
$C_3H_4F_4$	40723-63-5	21-046 /S1	1,1,2,2-Tetrafluoropropane	R254cb
$C_3H_4N_2$	288-32-4	33-003	1*H*-Imidazole	1,3-Diazole; Glyoxaline
	288-13-1	33-004	1*H*-Pyrazole	1,2-Diazole
$C_3H_4N_2O$	107-91-5	62-012	2-Cyanoacetamide	
$C_3H_4O_2$	57-57-8	47-001	2-Oxetanone	β-Propiolactone; Hydracrylolactone; USAN
	79-10-7	44-003 /B+S1	2-Propenoic acid	Acrylic acid; Acroleic acid
$C_3H_4O_3$	96-49-1	47-002 /B+S2	1,3-Dioxolan-2-one	Cyclic ethylene ester carbonic acid; Ethylene carbonate
C_3H_5Br	106-95-6	23-019	3-Bromo-1-propene	Allyl bromide
$C_3H_5Br_3$	96-11-7	23-020	1,2,3-Tribromopropane	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
C_3H_5Cl	107-05-1	22-021	3-Chloro-1-propene	3-Chloropropene; Allyl chloride
C_3H_5ClO	79-03-8	61-012	Propanoyl chloride	Propionyl chloride
$C_3H_5ClO_2$	96-34-4	61-013	Methyl chloroacetate	Methyl ester chloroacetic acid
$C_3H_5Cl_3$	96-18-4	22-022	1,2,3-Trichloropropane	
$C_3H_5D_3O_3$	7325-16-8	42-007	1,2,3-Propanetriol-O,O,O-d_3	Glycerol-O,O,O-d_3; Trideuteroglycerol
C_3H_5N	107-12-0	32-005 /B+S1	Propanenitrile	Propionitrile; Ethyl cyanide
C_3H_5NO	1738-36-9	62-129 /S1	Methoxyacetonitrile	
	79-06-1	62-013	2-Propenamide	Acrylamide
$C_3H_5NO_4$	2483-57-0	62-014	Methyl ester nitroacetic acid	Methyl nitroacetate
C_3H_5NS	542-85-8	64-005	Isothiocyanatoethane	Ethyl isothiocyanate
$C_3H_5N_2O$	497-25-6	62-175 /S2	2-Oxazolidinone	Dimethylene urethane; 2-Oxotetrahydro-1,3-oxazole
$C_3H_5NaO_2$	137-40-6	74-002	Sodium salt propanoic acid	Sodium propanoate; Natrium propionate
C_3H_6	75-19-4	12-001	Cyclopropane	Trimethylene
	115-07-1	13-002	1-Propene	Propylene
$C_3H_6Br_2$	78-75-1	23-021	1,2-Dibromopropane	Propylene bromide
	109-64-8	23-022 /B+S1+S2	1,3-Dibromopropane	Trimethylene bromide
$C_3H_6Cl_2$	78-87-5	22-023 /B+S1	1,2-Dichloropropane	Propylene chloride
	142-28-9	22-024 /B+S1+S2	1,3-Dichloropropane	Trimethylene dichloride
	594-20-7	22-025	2,2-Dichloropropane	Isopropylidene chloride
$C_3H_6Cl_2Si$	124-70-9	71-059 /S1	Dichloroethenylmethylsilane	Dichloromethylvinylsilane
$C_3H_6F_4N_2$	15403-25-5	64-006	N,N,N',N'-Tetrafluoro-1,2-propanediamine	
$C_3H_6I_2$	627-31-6	24-010 /S1	1,3-Di-iodopropane	
$C_3H_6N_2O_4$	595-49-3	62-015	2,2-Dinitropropane	
C_3H_6O	75-56-9	46-002	Methyloxirane	1,2-Epoxypropane; 1,2-Propylene oxide
	503-30-0	46-003	Oxetane	Trimethylene oxide
	123-38-6	43-003	Propanal	Propionaldehyde
	67-64-1	43-004 /B+S1	2-Propanone	Dimethyl ketone; Acetone
	107-18-6	42-008	2-Propen-1-ol	Allyl alcohol
$C_3H_6O_2$	646-06-0	46-004 /B+S1+S2	1,3-Dioxolane	
	109-94-4	45-002 /B+S1	Ethyl formate	Ethyl methanoate
	79-20-9	45-003 /B+S1	Methyl acetate	Methyl ethanoate
	79-09-4	44-004 /B+S1+ S2	Propanoic acid	Propionic acid; Methylacetic acid
$C_3H_6O_2S$	107-96-0	63-003	3-Mercaptopropanoic acid	3-Thiolpropionic acid; β-Thiolacetic acid
$C_3H_6O_3$	616-38-6	45-004 /B+S1+S2	Dimethyl carbonate	Methyl carbonate
	598-82-3	47-003	(R,S)-2-Hydroxypropanoic acid	Lactic acid (racemic)
	96-35-5	47-052 /S1	Methyl ester hydroxyacetic acid	Methyl glycolate
	110-88-3	46-005	1,3,5-Trioxane	*sym*-Trioxane
C_3H_6S	287-27-4	53-001	Thietane	Thiacyclobutane; Trimethylene sulfide
$C_3H_6S_3$	291-21-4	53-015 /S2	1,3,5-Trithiane	*s*-Trithiane; Thioform; Trimethylenetrisulfide; 1,3,5-Trithiacyclohexane
C_3H_7Br	106-94-5	23-023 /B+S1+S2	1-Bromopropane	Propyl bromide
	75-26-3	23-024 /B+S1	2-Bromopropane	Isopropyl bromide
C_3H_7Cl	540-54-5	22-026 /B+S2	1-Chloropropane	Propyl chloride
C_3H_7ClO	127-00-4	61-056 /S2	1-Chloro-2-propanol	α-Propylene chlorohydrin; 1-Chloroisopropyl alcohol
C_3H_7I	107-08-4	24-004 /B+S1	1-Iodopropane	Propyl iodide

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	75-30-9	24-011 /S1	2-Iodopropane	Isopropyl iodide
C_3H_7N	765-30-0	31-005	Cyclopropanamine	Cyclopropylamine
C_3H_7NO	68-12-2	62-016 /B+S1+S2	*N*,*N*-Dimethylformamide	*N*,*N*-Dimethylmethanamide
$C_3H_7NO_2$	51-79-6	62-017	Ethyl ester carbamic acid	Ethyl carbamate; Ethyl urethane
	108-03-2	62-130 /S1	1-Nitropropane	
$C_3H_7NO_3$	1712-64-7	62-018	1-Methylethyl ester nitric acid	Isopropyl nitrate
C_3H_8	74-98-6	11-005	Propane	
$C_3H_8N_2O_2$	4114-31-2	62-176 /S2	Ethyl ester hydrazinecarboxylic acid	Ethyl hydrazinocarboxylate
C_3H_8O	71-23-8	42-009 /B+S1+S2	1-Propanol	Propyl alcohol
	67-63-0	42-010 /B+S1+S2	2-Propanol	Isopropyl alcohol
$C_3H_8OS_2$	33577-16-1	63-009 /S2	(Methylsulfinyl)(methylthio)methane	(Methylthio) dimethylsulfoxide
$C_3H_8O_2$	109-87-5	41-002 /B+S1	Dimethoxymethane	2,4-Dioxapentane; Formaldehyde dimethyl acetal; Methylal
	109-86-4	47-004 /B+S2	2-Methoxyethanol	Methyl cellosolve; Glycol monomethyl ether
	57-55-6	42-011 /B+S1+S2	1,2-Propanediol	Propylene glycol
	504-63-2	42-126 /S2	1,3-Propanediol	1,3-Propylene glycol; Trimethylene glycol
$C_3H_8O_3$	56-81-5	42-012	1,2,3-Propanetriol	Glycerol; Glycyl alcohol; Glycerine
C_3H_8S	624-89-5	51-003	(Methylthio)ethane	Ethyl methyl sulfide
	107-03-9	52-003	1-Propanethiol	1-Propyl mercaptan
	75-33-2	52-004	2-Propanethiol	Isopropyl mercaptan
C_3H_9Al	75-24-1	73-005	Trimethylaluminum	
C_3H_9As	593-88-4	73-006	Trimethylarsine	
C_3H_9B	593-90-8	72-005	Trimethylborane	
$C_3H_9BO_3$	121-43-7	72-016 /S1	Trimethyl ester boric acid (H_3BO_3)	Trimethyl borate; Methyl borate
C_3H_9ClSi	75-77-4	71-060 /S1	Chlorotrimethylsilane	
C_3H_9Ga	1445-79-0	73-007	Trimethylgallium	
C_3H_9N	75-50-3	31-006	*N*,*N*-Dimethylmethanamine	Trimethylamine
	107-10-8	31-007 /B+S2	1-Propanamine	*n*-Propylamine
	75-31-0	31-008	2-Propanamine	Isopropylamine
C_3H_9NO	109-83-1	62-131 /S1	2-(Methylamino)ethanol	*N*-Methylethanolamine
$C_3H_{10}N_2$	10424-38-1	31-009	(*R*,*S*)-1,2-Propanediamine	1,2-Diaminopropane (racemic)
	109-76-2	31-066 /S2	1,3-Propanediamine	1,3-Trimethylenediamine
	1741-01-1	34-005	Trimethylhydrazine	
$C_3H_{12}BN$	75-22-9	72-006	Trimethylamineborane	*N*,*N*-Dimethylmethanamine compd. with borane (1:1)
C_3O_2	504-64-3	43-002	1,2-Propadiene-1,3-dione	Carbon suboxide
$C_4Br_2Cl_2F_6$	375-42-8	25-026	1,4-Dibromo-2,3-dichloro-1,1,2,3,4,4-hexafluorobutane	
C_4D_8O	1693-74-9	46-027 /S1	Tetrahydro-d_4-furan-d_4	Tetradeuterofuran
C_4F_8	115-25-3	21-007	Octafluorocyclobutane	Perfluorocyclobutane
C_4HClF_6	132186-30-2	25-048 /S1	4-Chloro-1,1,2,2,3,3-hexafluorocyclobutane	Rc-326d
$C_4HF_7O_2$	375-22-4	61-057 /S2	Heptafluorobutanoic acid	Perfluorobutanioc acid; Perfluorobutyric acid
C_4HF_9	375-17-7	21-047 /S1	1,1,1,2,2,3,3,4,4-Nonafluorobutane	R329cca
$C_4H_2F_8$	662-35-1	21-048 /S1	1,1,1,2,2,3,3,4- Octafluorobutane	R338ccb
	377-36-6	21-049 /S1	1,1,2,2,3,3,4,4-Octafluorobutane	R338cca
$C_4H_2O_3$	108-31-6	44-005 /B+S1	2,5-Furandione	(*Z*)-Butenedioic acid anhydride; Maleic anhydride
C_4H_3BrS	1003-09-4	64-032 /S1	2-Bromothiophene	
C_4H_3ClS	96-43-5	64-033 /S1	2-Chlorothiophene	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_4H_3Cl_3OS$	76619-91-5	64-007	*O*-Methyl ester 2,3,3-trichloro-2-propenethioic acid	*O*-Methyl ester trichlorothioacrylic acid; Methyl trichlorothioacrylate
$C_4H_3F_7$	662-00-0	21-050 /S1	1,1,1,2,2,3,3-Heptafluorobutane	R347ccd
$C_4H_4N_2$	110-61-2	32-006	Butanedinitrile	Succinonitrile; Ethylene dicyanide
	290-37-9	33-057 /S2	Pyrazine	1,4-Diazabenzene; *p*-Diazine
C_4H_4O	110-00-9	46-006	Furan	Furfuran; Tetrol
$C_4H_4O_4$	502-97-6	47-005	1,4-Dioxane-2,5-dione	*p*-Dioxane-2,5-dione; Glycolide; Diglycolide
C_4H_4S	110-02-1	53-002	Thiophene	Thiofuran
C_4H_5Cl	126-99-8	22-027	2-Chloro-1,3-butadiene	Chloroprene
$C_4H_5ClO_3$	2463-45-8	61-050 /S1	4-(Chloromethyl)-1,3-dioxolan-2-one	4-Chloromethyl carbonate
$C_4H_5ClO_2$	6214-28-4	61-014	(*E*)-3-Chloro-2-butenoic acid	*trans*-3-Chloro-2-butenoic acid; 3-Chlorocrotonic acid
	6213-90-7	61-015	(*Z*)-3-Chloro-2-butenoic acid	*cis*-3-Chloro-2-butenoic acid; 3-Chloroisocrotonic acid
$C_4H_5Cl_3O$	76-36-8	61-016	2,2,3-Trichlorobutanal	2,2,3-Trichlorobutyraldehyde; Butylchloral
$C_4H_5Cl_3O_2$	515-84-4	61-017	Ethyl trichloroacetate	Ethyl ester trichloroacetic acid
C_4H_5N	5500-21-0	32-007	Cyclopropanecarbonitrile	Cyclopropyl cyanide; Cyanocyclopropane
	126-98-7	32-008	2-Methyl-2-propenenitrile	Methacrylonitrile
	109-97-7	33-005	1*H*-Pyrrole	Azole
C_4H_5NO	3515-93-3	62-019	4-Oxobutanenitrile	β-Cyanopropionaldehyde
$C_4H_5NO_2$	105-34-0	62-132 /S1	Methyl ester cyanoacetic acid	Methyl cyanoacetate
	123-56-8	62-020	2,5-Pyrrolidinedione	Succinimide
C_4H_5NS	57-06-7	64-008	3-Isothiocyanato-1-propene	Allyl isothiocyanate
	3581-87-1	64-009	2-Methylthiazole	
C_4H_6	590-19-2	13-003	1,2-Butadiene	
	106-99-0	13-004	1,3-Butadiene	Vinylethylene; Divinyl; Erythrene
	107-00-6	13-005	1-Butyne	Ethylacetylene
	503-17-3	13-006	2-Butyne	Dimethylacetylene; Crotonylene
$C_4H_6Cl_2O_2$	535-15-9	61-018	Ethyl dichloroacetate	Ethyl ester dichloroacetic acid
$C_4H_6N_2$	616-47-7	33-047 /S1	1-Methyl-1*H*-imidazole	
	930-36-9	33-048 /S1	1-Methyl-1*H*-pyrazole	
C_4H_6O	1191-99-7	46-007 /B+S2	2,3-Dihydrofuran	
	4170-30-3	43-005	2-Butenal	Crotonoaldehyde
	123-73-9	43-072 /S2	(*E*)-2-Butenal	*trans*-Crotonaldehyde; (*E*)-Crotonaldehyde
$C_4H_6O_2$	107-93-7	44-006 /B+S1	(*E*)-2-Butenoic acid	*trans*-2-Butenoic acid; Crotonic acid
	1759-53-1	44-040 /S2	Cyclopropane carboxylic acid	Carboxycyclopropane
	96-48-0	47-006 /B+S1	2(3*H*)-Dihydrofuranone	γ-Butyrolactone; 4-Butanolide
	108-05-4	45-005 /B+S1	Ethenyl acetate	Vinyl acetate; Ethenyl ethanoate
	96-33-3	45-006	Methyl propenoate	Methyl acrylate
	79-41-4	44-007	2-Methyl-2-propenoic acid	Methacrylic acid; α-Methacrylic acid
$C_4H_6O_3$	108-24-7	44-008	Acetic acid anhydride	Acetic anhydride; Ethanoic acid anhydride
	3041-16-5	47-076 /S2	1,4-Dioxan-2-one	2-Oxo-1,4-dioxanone; δ-Lactone

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	108-32-7	47-007 /B+S1+S2	4-Methyl-1,3-dioxolan-2-one	Cyclic propylene ester carbonic acid; Propylene carbonate
$C_4H_6O_4$	553-90-2	45-131 /S1	Dimethyl ester ethanedioic acid	Dimethyl ethanedioate; Dimethyl oxalate
	931-40-8	47-077 /S2	4-Hydroxymethyl-1,3-dioxolan-2-one	Glycerol cyclic 1,2-carbonate; Glycerinecarbonate; (Hydroxymethyl)ethylene ester carbonic acid
C_4H_6Te	63000-06-6	73-035 /S1	1,1′-Tellurobis(ethene)	Divinyltellurium
C_4H_7ClO	141-75-3	61-019	Butanoyl chloride	Butyryl chloride
	79-30-1	61-020	2-Methylpropanoyl chloride	2-Methylpropionyl chloride; Isobutyryl chloride
$C_4H_7ClO_2$	105-39-5	61-021	Ethyl chloroacetate	Ethyl ester chloroacetic acid
$C_4H_7Cl_2NSi$	1071-21-2	71-005	3-(Dichloromethylsilyl)propanenitrile	3-(Dichloromethylsilyl) propionitrile; Dichloro-(2-cyanethyl) methylsilane
$C_4H_7LiO_2$	25179-23-1	74-025 /S1	Lithium salt 2-methylpropanoic acid	Lithium isobutyrate
C_4H_7N	109-74-0	32-009	Butanenitrile	Butyronitrile; Propyl cyanide
	78-82-0	32-010	2-Methylpropanenitrile	2-Methylpropionitrile; Isobutyronitrile; Isopropyl cyanide
C_4H_7NO	62957-60-2	62-133 /S1	Ethoxyacetonitrile	
	110-67-8	62-021	3-Methoxypropionitrile	
	616-45-5	62-022	2-Pyrrolidinone	2-Pyrrolidone; γ-Butyrolactam
$C_4H_7NO_2$	5259-97-2	62-134 /S1+S2	Tetrahydro-2*H*-1,3-oxazin-2-one	
$C_4H_7NaO_2$	156-54-7	74-003	Sodium salt butanoic acid	Sodium butanoate; Natrium butyrate
$C_4H_7O_2Tl$	63424-49-7	74-026 /S1	Thallium(1+) salt butanoic acid	Thallium(I) butyrate
C_4H_8	106-98-9	13-007 /B+S1	1-Butene	
	624-64-6	13-008	(*E*)-2-Butene	*trans*-2-Butene; *trans*-Dimethylethylene
	590-18-1	13-009	(*Z*)-2-Butene	*cis*-2-Butene; *cis*-Dimethylethylene
	287-23-0	12-002	Cyclobutane	Tetramethylene
	115-11-7	13-010	2-Methyl-1-propene	Isobutene
$C_4H_8Br_2$	110-52-1	23-041 /S1+S2	1,4-Dibromobutane	
$C_4H_8Cl_2$	616-21-7	22-051 /S1	1,2-Dichlorobutane	
	110-56-5	22-028 /B+S1+S2	1,4-Dichlorobutane	Tetramethylene dichloride
$C_4H_8Cl_2O$	111-44-4	61-022	1,1′-Oxybis(2-chloroethane)	Bis(2-chloroethyl) ether; β,β'-Dichlorodiethyl ether; Chlorex
$C_4H_8N_2$	1606-49-1	33-049 /S1	1,4,5,6-Tetrahydropyrimidine	
$C_4H_8N_2O_7$	693-21-0	62-177 /S2	2,2′-Oxybis(ethanol) dinitrate	Diglycol dinitrate; Dinitrodiglycol
C_4H_8O	123-72-8	43-006	Butanal	Butyraldehyde
	78-93-3	43-007 /B+S1+S2	2-Butanone	Ethyl methyl ketone
	106-88-7	46-008 /B+S1	Ethyloxirane	1,2-Epoxybutane; 1,2-Butylene oxide
	116-11-0	41-003	2-Methoxy-1-propene	Isopropenyl methyl ether
	109-99-9	46-009 /B+S1+S2	Tetrahydrofuran	Oxolane; Tetramethylene oxide
$C_4H_8O_2$	107-92-6	44-009	Butanoic acid	Butyric acid; Ethylacetic acid; Propylformic acid
	505-22-6	46-010 /B+S2	1,3-Dioxane	*m*-Dioxane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	123-91-1	46-011 /B+S1+S2	1,4-Dioxane	*p*-Dioxane; 1,4-Diethylene dioxide; Dioxyethylene ether; Diethylene ether
	141-78-6	45-007 /B+S1	Ethyl acetate	Ethyl ethanoate
	554-12-1	45-008 /B+S1	Methyl propanoate	Methyl propionate
	79-31-2	44-010 /B+S1	2-Methylpropanoic acid	Isobutyric acid
	110-74-7	45-009 /B+S1	Propyl formate	Propyl methanoate
$C_4H_8O_2S$	126-33-0	63-004 /B+S1	Tetrahydrothiophene 1,1-dioxide	Tetramethylene sulfone; Sulfolane
$C_4H_8O_3$	542-59-6	47-053 /S1	1,2-Ethanediol monoacetate	Ethylene glycol monoacetate; 2-Hydroxyethyl acetate
	623-53-0	45-161 /S2	Ethyl methyl carbonate	Ethyl methyl ester carbonic acid
	6290-49-9	47-054 /S1	Methyl ester methoxyacetic acid	Methyl methoxyacetate
$C_4H_8O_4$	293-30-1	46-012	1,3,5,7-Tetraoxacyclooctane	1,3,5,7-Tetroxocane
C_4H_8S	110-01-0	53-003	Tetrahydrothiophene	Thiolane; Tetramethylenesulfide
$C_4H_8S_2$	505-23-7	53-004	1,3-Dithiane	*m*-Dithiane
	505-29-3	53-005	1,4-Dithiane	*p*-Dithiane
C_4H_9Br	109-65-9	23-025 /B+S1+S2	1-Bromobutane	*n*-Butyl bromide
	78-77-3	23-026 /B+S1	1-Bromo-2-methylpropane	Isobutyl bromide
	507-19-7	23-027 /B+S1	2-Bromo-2-methylpropane	*tert*-Butyl bromide
C_4H_9Cl	109-69-3	22-029 /B+S1+S2	1-Chlorobutane	*n*-Butyl chloride
	78-86-4	22-052 /S1	2-Chlorobutane	*sec*-Butyl chloride
	513-36-0	22-030 /B+S1	1-Chloro-2-methylpropane	Isobutyl chloride
	507-20-0	22-031	2-Chloro-2-methylpropane	*tert*-Butyl chloride
C_4H_9I	542-69-8	24-012 /S1	1-Iodobutane	Butyl iodide
	513-48-4	24-013 /S1	2-Iodobutane	*sec*-Butyl iodide
	513-38-2	24-005 /B+S1	1-Iodo-2-methylpropane	Isobutyl iodide
C_4H_9N	123-75-1	33-006	Pyrrolidine	Tetrahydropyrrole; Azolidine
C_4H_9NO	96-29-7	62-023	2-Butanone oxime	Ethyl methyl ketoxime (unspec. isomer)
	127-19-5	62-024	*N*,*N*-Dimethylacetamide	
	625-50-3	62-025	*N*-Ethylacetamide	*N*-Ethylethanamide
	1187-58-2	62-026	*N*-Methylpropanamide	*N*-Methylpropionamide
	110-91-8	62-027	Morpholine	Tetrahydro-4*H*-1,4-oxazine; Diethylenimide oxide
C_4H_{10}	106-97-8	11-006	Butane	
	75-28-5	11-007	2-Methylpropane	Isobutane; Trimethylmethane
$C_4H_{10}Cl_2Si$	1719-53-5	71-006	Dichlordiethylsilane	
$C_4H_{10}Hg$	627-44-1	73-008	Diethylmercury	
$C_4H_{10}N_2$	110-85-0	33-007 /B+S1	Piperazine	Hexahydropyrazine; Perhydro-1,4-diazine; Diethylenediamine
$C_4H_{10}O$	71-36-3	42-013 /B+S1+S2	1-Butanol	Butyl alcohol
	78-92-2	42-014 /B+S1+S2	2-Butanol	*sec*-Butyl alcohol; Methyl ethyl carbinol (unspec. chirality)
	15892-23-6	42-015	(*R*,*S*)-2-Butanol	*sec*-Butyl alcohol; Methyl ethyl carbinol (racemic)
	4221-99-2	42-016	(*S*)-2-Butanol	*D*-*sec*-Butyl alcohol; *D*-Methylethylcarbinol
	557-17-5	41-004	1-Methoxypropane	Methyl propyl ether
	598-53-8	41-005	2-Methoxypropane	Methyl 1-methylethyl ether; Isopropyl methyl ether
	78-83-1	42-017 /B+S1+S2	2-Methyl-1-propanol	Isobutyl alcohol
	75-65-0	42-018 /B+S2	2-Methyl-2-propanol	*tert*-Butyl alcohol; Trimethyl carbinol

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	60-29-7	41-006	1,1′-Oxybis(ethane)	Diethyl ether; Ethyl ether; Ethyl oxide; Diethyl oxide
$C_4H_{10}O_2$	26171-83-5	42-108 /S1+S2	(±)-1,2-Butanediol	
	107-88-0	42-019 /B+S1+S2	1,3-Butanediol	1,3-Butylene glycol
	110-63-4	42-020 /B+S2	1,4-Butanediol	1,4-Butylene glycol; Tetramethylene glycol
	513-85-9	42-021 /B+ S2	2,3-Butanediol	2,3-Butylene glycol
	110-71-4	41-007 /B+S1+S2	1,2-Dimethoxyethane	2,5-Dioxahexane; Ethylene glycol dimethyl ether; Monoglyme; GDME
	110-80-5	47-008 /B+S1	2-Ethoxyethanol	3-Oxa-1-pentanol; Ethyl cellosolve; Ethylene glycol monoethyl ether
$C_4H_{10}O_2Se$	27974-49-8	73-009	2,2′-Selenodiethanol	β-Selenium diglycol
$C_4H_{10}O_3$	111-46-6	47-009 /B+S1+S2	2,2′-Oxybis(ethanol)	1,5-Dihydroxy-3-oxapentane; 2,2′-Dihydroxydiethyl ether; Diethylene glycol
$C_4H_{10}O_4$	149-32-6	42-022	(R∗,S∗)-1,2,3,4-Butanetetrol	Erythro-1,2,3,4-butanetetrol; Erythritol
$C_4H_{10}S$	109-79-5	52-005	1-Butanethiol	1-Butyl mercaptan
	513-53-1	52-006	2-Butanethiol	2-Butyl mercaptan; *sec*-Butyl mercaptan
	513-44-0	52-007	2-Methyl-1-propanethiol	Isobutyl mercaptan
	75-66-1	52-008	2-Methyl-2-propanethiol	*tert*-Butyl mercaptan
	3877-15-4	51-004	1-(Methylthio)propane	Methyl propyl sulfide
	1551-21-9	51-005	2-(Methylthio)propane	Methyl 1-methylethyl sulfide; Isopropyl methyl sulfide
	352-93-2	51-006	1,1′-Thiobis(ethane)	Diethyl sulfide
$C_4H_{10}S_2$	110-81-6	51-007	3,4-Dithiahexane	Diethyl disulfide; Ethyl disulfide
$C_4H_{10}Te$	627-54-3	73-036 /S1	Diethyltelluride	
$C_4H_{10}Zn$	557-20-0	73-010	Diethylzinc	
$C_4H_{11}N$	109-73-9	31-010 /B+S2	1-Butanamine	*n*-Butylamine
	109-89-7	31-011 /B+S1	*N*-Ethylethanamine	Diethylamine
	78-81-9	31-012	2-Methyl-1-propanamine	Isobutylamine
	75-64-9	31-013	2-Methyl-2-propanamine	*tert*-Butylamine
$C_4H_{11}NO$	124-68-5	62-028 /B+S1+S2	2-Amino-2-methyl-1-propanol	Isobutanolamine
	3710-84-7	62-029	*N*,*N*-Diethylhydroxylamine	
	108-01-0	62-135 /S1	2-(Dimethylamino)ethanol	Dimethylethanolamine
	110-73-6	62-136 /S1	2-(Ethylamino)ethanol	Ethylethanolamine
	5332-73-0	62-030	3-Methoxy-1-propanamine	3-Methoxypropylamine; 4-Oxapentanamine
$C_4H_{11}NO_2$	929-06-6	62-137 /S1	2-(2-Aminoethoxy)ethanol	Diglycolamine
	115-69-5	62-031	2-Amino-2-methyl-1,3-propanediol	
	111-42-2	62-138 /S1	2,2′-Iminobis(ethanol)	Diethanolamine; 2-(2-Hydroxyethylamino)ethanol
$C_4H_{11}NO_3$	77-86-1	62-032	2-Amino-2-(hydroxymethyl)-1,3-propanediol	Trometamol
$C_4H_{12}CdSe$	143481-65-6	73-011	Dimethyl[selenobis(methane)]cadmium	
$C_4H_{12}CdTe$	143481-66-7	73-012	Dimethyl[tellurobis(methane)]cadmium	
$C_4H_{12}Ge$	865-52-1	73-013	Tetramethylgermane	
$C_4H_{12}N_2$	811-93-8	31-014	2-Methyl-1,2-propanediamine	1,2-Diamino-2-methylpropane
$C_4H_{12}O_4Si$	681-84-5	71-007	Tetramethyl ester silicic acid	Tetramethyl orthosilicate; Tetramethoxysilane
$C_4H_{12}Pb$	75-74-1	73-014	Tetramethylplumbane	Tetramethyllead
$C_4H_{12}SZn$	91071-61-3	73-037 /S1	Dimethyl[thiobis(methane)]zinc	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_4H_{12}SeZn$	108430-95-1	73-015	Dimethyl[selenobis(methane)]zinc	Complex dimethylzinc with dimethylselenium
$C_4H_{12}Si$	75-76-3	71-008	Tetramethylsilane	
$C_4H_{12}Sn$	594-27-4	73-016	Tetramethylstannane	Tetramethyltin
$C_4H_{12}TeZn$	127283-03-8	73-017	Dimethyl[tellurobis(methane)]zinc	Complex dimethylzinc with dimethyltellurium
$C_4H_{13}N_3$	111-40-0	31-015 /B+S1	*N*-(2-Aminoethyl)-1,2-ethanediamine	Diethylenetriamine
C_4NiO_4	13463-39-3	02-029	Nickel carbonyl	
$C_5F_{11}N$	836-77-1	64-010	Undecafluoropiperidine	Perfluoropiperidine
C_5F_{12}	678-26-2	21-008	Dodecafluoropentane	Perfluoropentane
$C_5F_{13}N$	758-48-5	64-011	1,1,2,2,2-Pentafluoro-*N*-(pentafluoroethyl)-*N*-(trifluoromethyl)-ethanamine	
$C_5H_3F_7O_2$	356-24-1	61-023	Methyl heptafluorobutanoate	Methyl ester heptafluorobutanoic acid; Methyl perfluorobutyrate
$C_5H_4N_4$	275-02-5	33-050 /S1	[1,2,4]Triazolo[1,5-*a*]pyrimidine	
$C_5H_4O_2$	98-01-1	47-010 /B+S1	2-Furancarboxaldehyde	Furfural; Pyromucic aldehyde; Furfuraldehyde
$C_5H_5Cl_3OS$	76619-92-6	64-034 /S1	*O*-Ethyl ester 2,3,3-trichloro-2-propenethioic acid	*O*-Ethyl ester trichlorothioacrylate
$C_5H_5Cl_3O_2$	6304-34-3	61-024	2-Propenyl trichloroacetate	2-Propenyl ester trichloroacetic acid; Allyl trichloroacetate
C_5H_5N	16955-35-4	32-011	Bicyclo[1.1.0]butane-1-carbonitrile	1-Bicyclobutyl cyanide; 1-Cyanobicyclobutane
	110-86-1	33-008 /B+S1	Pyridine	Azine
C_5H_6	542-92-7	14-098 /S1	1,3-Cyclopentadiene	
$C_5H_6Cl_2O_2$	30895-77-3	61-025	2-Propenyl dichloroacetate	2-Propenyl ester dichloroacetic acid; Allyl dichloroacetate
$C_5H_6N_2$	7321-55-3	32-012	Dimethylpropanedinitrile	2,2-Dicyanopropane; Dimethylmalononitrile
	544-13-8	32-013	Pentanedinitrile	1,3-Dicyanopropane; Glutaronitrile; Trimethylenedicyanide
C_5H_6O	534-22-5	46-013	2-Methylfuran	Sylvan
$C_5H_6O_2$	98-00-0	47-011	2-Furanmethanol	Furfuryl alcohol; Furyl carbinol
C_5H_6S	554-14-3	53-006	2-Methylthiophene	
	616-44-4	53-007	3-Methylthiophene	
$C_5H_7ClO_2$	2916-14-5	61-026	2-Propenyl chloroacetate	2-Propenyl ester chloroacetic acid; Allyl chloroacetate
$C_5H_7Cl_3O_2$	13313-91-2	61-027	Propyl trichloroacetate	Propyl ester trichloroacetic acid
C_5H_7N	4426-11-3	32-014	Cyclobutanecarbonitrile	Cyclobutyl cyanide; Cyanocyclobutane
	96-54-8	33-009	1-Methyl-1*H*-pyrrole	
$C_5H_7NO_2$	105-56-6	62-033	Ethyl ester cyanoacetic acid	Ethyl cyanoacetate
	14618-77-0	62-139 /S1	Methyl ester 2-cyanopropanoic acid	Methyl 2-cyanopropionate
C_5H_8	142-29-0	14-001	Cyclopentene	
	78-79-5	13-011	2-Methyl-1,3-butadiene	Isoprene
	598-25-4	13-012	3-Methyl-1,2-butadiene	
	1120-56-5	12-003	Methylenecyclobutane	
	591-95-7	13-013	1,2-Pentadiene	
	2004-70-8	13-014	(*E*)-1,3-Pentadiene	*trans*-1,3-Pentadiene
	1574-41-0	13-015	(*Z*)-1,3-Pentadiene	*cis*-1,3-Pentadiene
	591-93-5	13-016	1,4-Pentadiene	
	591-96-8	13-017	2,3-Pentadiene	
	157-40-4	12-004	Spiropentane	Spirocyclane; Cyclopropanespirocyclopropane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_5H_8Br_4$	3229-00-3	23-028	1,3-Dibromo-2,2-bis(bromomethyl)propane	2,2-Bis(bromomethyl)-1,3-dibromopropane; Pentaerythrityl tetrabromide
$C_5H_8Cl_2O$	78-71-7	61-028	3,3-Bis(chloromethyl)oxetane	3,3-Bis(chloromethyl) oxacyclobutane
$C_5H_8Cl_2O_2$	6628-21-3	61-029	Ethyl 2,3-dichloropropanoate	Ethyl ester 2,3-dichloropropanoic acid
	37587-81-8	61-030	Propyl dichloroacetate	Propyl ester dichloroacetic acid
$C_5H_8Cl_4$	3228-99-7	22-032	1,3-Dichloro-2,2-bis(chloromethyl)propane	2,2-Bis(chloromethyl)-1,3-dichloropropane; Pentaerythrityl tetrachloride
$C_5H_8F_4$	338-23-8	21-009	1,3-Difluoro-2,2-bis(fluoromethyl)propane	2,2-Bis(fluoromethyl)-1,3-difluoropropane; Pentaerythrityl tetrafluoride
$C_5H_8N_2$	7098-07-9	33-051 /S1	1-Ethyl-1*H*-imidazole	
	2817-71-2	33-052 /S1	1-Ethyl-1*H*-pyrazole	
C_5H_8O	120-92-3	43-008 /B+S1+S2	Cyclopentanone	
$C_5H_8O_2$	80-62-6	45-010	Methyl 2-methyl-2-propenoate	Methyl methacrylate
	123-54-6	43-009 /B+S1	2,4-Pentanedione	Acetylacetone; Diacetylmethane
	591-87-7	45-011	2-Propenyl acetate	2-Propenyl ethanoate; Allyl acetate
	542-28-9	47-012	Tetrahydro-2*H*-pyran-2-one	δ-Valerolactone; 5-Pentanolide
$C_5H_8O_3$	4437-85-8	47-078 /S2	4-Ethyl-1,3-dioxolan-2-one	1,2-Butylene carbonate; Cyclic ethylethylene estercarbonic acid
	105-45-3	47-055 /S1	Methyl ester 3-oxobutanoic acid	Methyl acetoacetate
$C_5H_8O_4$	108-59-8	45-132 /S1+S2	Dimethyl ester propanedioic acid	Dimethyl malonate
	110-94-1	44-041 /S2	Pentanedioic acid	Glutaric acid; 1,3-Propanedicarboxylic acid
C_5H_9Cl	930-28-9	22-053 /S1	Chlorocyclopentane	Cyclopentyl chloride
C_5H_9ClO	638-29-9	61-031	Pentanoyl chloride	Valeryl chloride
$C_5H_9ClO_2$	535-13-7	61-032	Ethyl 2-chloropropanoate	Ethyl ester 2-chloropropanoic acid; Ethyl α-chloropropionate
	5396-24-7	61-033	Propyl chloroacetate	Propyl ester chloroacetic acid
C_5H_9N	630-18-2	32-015	2,2-Dimethylpropanenitrile	2-Cyano-2-methylpropane; Pivalonitrile; Trimethylacetonitrile
	110-59-8	32-016	Pentanenitrile	Valeronitrile; Butyl cyanide
C_5H_9NO	76474-09-4	62-140 /S1	2-Methoxy-2-methylpropanenitrile	2-Methoxy-2-methylpropionitrile
	872-50-4	62-034	1-Methyl-2-pyrrolidinone	1-Methyl-2-pyrrolidone
	675-20-7	62-035	2-Piperidinone	δ-Valerolactam; 2-Piperidone
$C_5H_9NO_2$	20721-78-2	62-141 /S1	4-Methyl-3-morpholinone	4-Methyl-3-oxomorpholine
C_5H_{10}	287-92-3	12-005	Cyclopentane	Pentamethylene
	563-46-2	13-018	2-Methyl-1-butene	
	513-35-9	13-019	2-Methyl-2-butene	Trimethylethylene; β-Isoamylene
	563-45-1	13-020	3-Methyl-1-butene	Isopropylethylene; α-Isoamylene
	109-67-1	13-021 /B+S1	1-Pentene	
	109-68-2	13-022	2-Pentene	β-Amylene; Methylethylethylene (unspecified stereoisomer)
	646-04-8	13-023	(*E*)-2-Pentene	*trans*-2-Pentene; *trans*−β-Amylene; *trans*-Methylethylethylene

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	627-20-3	13-024	(*Z*)-2-Pentene	*cis*-2-Pentene; *cis*−*β*-Amylene; *cis*-Methylethylethylene
$C_5H_{10}Br_2$	111-24-0	23-044 /S2	1,5-Dibromopentane	Pentamethylene dibromide
$C_5H_{10}Cl_2$	628-76-2	22-033 /B+S1+S2	1,5-Dichloropentane	Pentamethylene dichloride
$C_5H_{10}N_2$	1738-25-6	34-006	3-(Dimethylamino)-propanenitrile	3-(Dimethylamino)-propionitrile
$C_5H_{10}O$	96-41-3	42-023 /B+S1	Cyclopentanol	Cyclopentyl alcohol
	630-19-3	43-010 /B+S1	2,2-Dimethylpropanal	Pivalaldehyde; Trimethylacetaldehyde
	563-80-4	43-011	3-Methyl-2-butanone	Isopropyl methyl ketone
	115-18-4	42-024	2-Methyl-3-buten-2-ol	
	110-62-3	43-012	Pentanal	Valeraldehyde; Pentyl aldehyde; Amyl aldehyde
	107-87-9	43-013 /B+S2	2-Pentanone	Methyl propyl ketone
	96-22-0	43-014	3-Pentanone	Diethyl ketone; Metacetone; Ethyl propionyl; Propione
	142-68-7	46-014 /B+S1+S2	Tetrahydropyran	Oxane; Pentamethylene oxide
$C_5H_{10}O_2$	592-84-7	45-012 /B+S1	Butyl formate	Butyl methanoate
	75-98-9	44-037 /S1+S2	2,2-Dimethylpropanoic acid	Trimethylacetic acid; Pivalic acid
	505-65-7	46-015	1,3-Dioxepane	*m*-Dioxepane
	105-37-3	45-013 /B+S1	Ethyl propanoate	Ethyl propionate
	623-42-7	45-014	Methyl butanoate	Methyl butyrate
	503-74-2	44-011	3-Methylbutanoic acid	Isovaleric acid
	108-21-4	45-016	1-Methylethyl acetate	Isopropyl acetate; 1-Methylethyl ethanoate
	547-63-7	45-015	Methyl 2-methylpropanoate	Methyl isobutyrate
	542-55-2	45-017	2-Methylpropyl formate	2-Methylpropyl methanoate; Isobutyl formate
	109-52-4	44-012	Pentanoic acid	Valeric acid
	109-60-4	45-018 /B+S1+S2	Propyl acetate	Propyl ethanoate
	97-99-4	47-013	Tetrahydro-2-furanmethanol	Tetrahydrofurfuryl alcohol
$C_5H_{10}O_3$	105-58-8	45-019 /B+S1+S2	Diethyl carbonate	Ethyl carbonate
	110-49-6	47-014 /B+S1	2-Methoxyethanol acetate	2-Methoxyethyl acetate
$C_5H_{10}O_5$	16528-92-0	46-016	1,3,5,7,9-Pentoxecane	Pentoxane
$C_5H_{10}S$	1679-07-8	52-009	Cyclopentanethiol	Cyclopentyl mercaptan
	1795-09-1	53-008	2-Methyltetrahydrothiophene	2-Methylthiolane; 2-Methylcyclothiapentane
	4740-00-5	53-009	3-Methyltetrahydrothiophene	3-Methylthiolane; 3-Methylcyclothiapentane
	1613-51-0	53-010	Tetrahydro-2*H*-thiopyran	Thiacyclohexane; Pentamethylene sulfide
$C_5H_{11}Br$	107-82-4	23-029	1-Bromo-3-methylbutane	Isoamyl bromide
	110-53-2	23-030 /B+S1+S2	1-Bromopentane	*n*-Amyl bromide
$C_5H_{11}Cl$	107-84-6	22-034	1-Chloro-3-methylbutane	Isoamyl chloride
	543-59-9	22-054 /S1+S2	1-Chloropentane	Pentyl chloride; Amyl chloride
$C_5H_{11}I$	541-28-6	24-006	1-Iodo-3-methylbutane	Isoamyl iodide
	628-17-1	24-014 /S1	1-Iodopentane	Pentyl iodide; Amyl iodide
$C_5H_{11}N$	1003-03-8	31-016	Cyclopentanamine	Cyclopentylamine
	120-94-5	33-010	1-Methylpyrrolidine	*N*-Methylpyrrolidine
	34375-89-8	33-011	3-Methylpyrrolidine	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	110-89-4	33-012 /B+S1	Piperidine	Pentamethylenimine; Hexahydropyridine; Perhydroazine
$C_5H_{11}NO$	2675-88-9	62-036	*N*,2-Dimethylpropanamide	*N*-Methylisobutyramide
	17794-44-4	62-037	*N*-Methylbutanamide	*N*-Methylbutyramide
	1118-69-0	62-038	*N*–1–Methylethyl acetamide	*N*–1–Methylethyl ethanamide; *N*-Isopropylacetamide
	5331-48-6	62-039	*N*-Propylacetamide	*N*-Propylethanamide
$C_5H_{11}NO_2$	7148-06-3	62-142 /S1	Methyl ester *N*,*N*-dimethylglycine	Methyl ester *N*,*N*-dimethylaminoacetic acid
C_5H_{12}	463-82-1	11-008	2,2-Dimethylpropane	Neopentane; Tetramethylmethane
	78-78-4	11-009	2-Methylbutane	Isopentane
	109-66-0	11-010 /B+S2	Pentane	
$C_5H_{12}N_2O$	634-95-7	62-143 /S1	*N*,*N*-Diethylurea	1,1-Diethylurea
	632-22-4	62-040 /B+S2	Tetramethylurea	
$C_5H_{12}O$	75-84-3	42-109 /S1+S2	2,2-Dimethyl-1-propanol	Neopentyl alcohol
	628-32-0	41-008	1-Ethoxypropane	Ethyl propyl ether
	628-28-4	41-009 /B+S1	1-Methoxybutane	Butyl methyl ether
	1634-04-4	41-010 /B+S2	2-Methoxy-2-methylpropane	1,1-Dimethylethyl methyl ether; *tert*-Butyl methyl ether
	137-32-6	42-025 /B+S1+S2	2-Methyl-1-butanol	*sec*-Butyl carbinol
	75-85-4	42-026 /B+S1+S2	2-Methyl-2-butanol	*tert*-Amyl alcohol; *tert*-Pentyl alcohol; Dimethyl ethyl carbinol
	123-51-3	42-027 /B+S1+S2	3-Methyl-1-butanol	Isopentyl alcohol; Isoamyl alcohol
	598-75-4	42-028 /B+S1+S2	3-Methyl-2-butanol	*sec*-Isoamyl alcohol
	71-41-0	42-029 /B+S1+S2	1-Pentanol	*n*-Amyl alcohol
	6032-29-7	42-030 /B+S1+S2	2-Pentanol	*sec*-Amyl alcohol; Methyl propyl carbinol
	584-02-1	42-031 /B+S1+S2	3-Pentanol	1-Ethyl-1-propanol; Diethyl carbinol
$C_5H_{12}O_2$	77-76-9	41-011	2,2-Dimethoxypropane	Acetone dimethyl acetal
	126-30-7	42-032	2,2-Dimethyl-1,3-propanediol	
	5137-45-1	41-012	1-Ethoxy-2-methoxyethane	2,5-Dioxaheptane; Ethylene glycol ethyl ether methyl ether
	462-95-3	41-049 /S1	1,1′-[Methylenebis(oxy)]bis(ethane)	3,5-Dioxaheptane; Diethoxymethane; Formaldehyde diethyl acetal
	109-59-1	47-015 /B+S1	2-(1-Methylethoxy)ethanol	4-Methyl-3-oxa-1-pentanol; 2-Isopropoxyethanol; Ethylene glycol monoisopropyl ether
	111-29-5	42-033 /B+S2	1,5-Pentanediol	
	2807-30-9	47-016 /B+S1	2-Propoxyethanol	3-Oxa-1-hexanol; Ethylene glycol monopropyl ether; Propyl cellosolve
$C_5H_{12}O_3$	111-77-3	47-017	2-(2-Methoxyethoxy)ethanol	Diethylene glycol monomethyl ether
$C_5H_{12}S$	4110-50-3	51-008	1-(Ethylthio)propane	Ethyl propyl sulfide
	1679-09-0	52-010	2-Methyl-2-butanethiol	2-Methyl-2-butyl mercaptan; *tert*-Amyl mercaptan
	541-31-1	52-011	3-Methyl-1-butanethiol	3-Methylbutyl mercaptan; Isopentyl mercaptan; Isoamyl mercaptan
	2084-18-6	52-012	3-Methyl-2-butanethiol	3-Methyl-2-butyl mercaptan; *sec*-Isoamyl mercaptan
	6163-64-0	51-009	2-Methyl-2-(methylthio)propane	1,1-Dimethylethyl methyl sulfide; *tert*-Butyl methyl sulfide
	628-29-5	51-010	1-(Methylthio)butane	Butyl methyl sulfide

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	10359-64-5	51-011	2-(Methylthio)butane	3-Methyl-2-thiapentane; Methyl 1-methylpropyl sulfide; *sec*-Butyl methyl sulfide
	110-66-7	52-013	1-Pentanethiol	1-Pentyl mercaptan
	6156-25-8	51-012 /B+S2	Tetrakis(methylthia)methane	Tetramethyl ester tetrathiacarbonic acid
$C_5H_{12}Si$	2295-12-7	71-009	1,1-Dimethylsilacyclobutane	
	754-05-2	71-010 /B+S1	Ethenyltrimethylsilane	Trimethylvinylsilane
$C_5H_{13}N$	996-35-0	31-046 /S1	*N*,*N*-Dimethyl-2-propanamine	Isopropyldimethylamine
	616-39-7	31-017	*N*-Ethyl-*N*-methylethanamine	*N*-Methyldiethylamine; *N*,*N*-Diethylmethylamine
	110-58-7	31-018 /B+S2	1-Pentanamine	Pentylamine; *n*-Amylamine
$C_5H_{13}NO$	2893-43-8	62-041	2-(Ethylmethylamino)ethanol	*N*,*N*-Ethylmethylethanolamine
	16369-21-4	62-144 /S1	2-(Propylamino)ethanol	Propylethanolamine
$C_5H_{13}NO_2$	105-59-9	62-145 /S1+S2	2,2′-(Methylimino)bis(ethanol)	Methyldiethanolamine; 2-[(2-Hydroxyethyl) methylamino]ethanol
$C_5H_{13}NSi$	2116-90-7	71-061 /S1	1-(Trimethylsilyl)aziridine	Trimethylsilylethyleneimine
$C_5H_{14}N_2$	109-55-7	31-019	*N*,*N*-Dimethyl-1,3-propanediamine	*N*,*N*-Dimethylpropylenediamine
C_6BrF_5	344-04-7	25-027	Bromopentafluorobenzene	
$C_6Br_2Cl_3F_9$	85131-86-8	25-028	1,6-Dibromo-2,3,5-trichloro-1,1,2,3,4,4, 5,6,6-nonafluorohexane	
C_6ClF_5	344-07-0	25-029	Chloropentafluorobenzene	
$C_6Cl_3F_3$	319-88-0	25-030	1,3,5-Trichloro-2,4,6-trifluorobenzene	
C_6D_6	1076-43-3	14-002	Benzene-d_6	Hexadeuterobenzene
C_6D_{12}	1735-17-7	12-006	Cyclohexane-d_{12}	Dodecadeuterocyclohexane
$C_6F_5NO_2$	880-78-4	64-012	Pentafluoronitrobenzene	
C_6F_6	392-56-3	21-010 /B+S1+S2	Hexafluorobenzene	Perfluorobenzene
C_6F_{12}	2070-70-4	21-051 /S1	1,1,1,2,3,4,5,5,5-Nonafluoro-4-(trifluoromethyl)-2-pentene	Perfluoro-4-methyl-2-pentene
C_6F_{14}	355-42-0	21-011	Tetradecafluorohexane	Perfluorohexane
$C_6F_{15}N$	359-70-6	64-013	1,1,2,2,2-Pentafluoro-*N*,*N*-bis(pentafluoroethyl)ethanamine	
C_6HCl_5	608-93-5	22-055 /S1	Pentachlorobenzene	
C_6HF_5	363-72-4	21-012	Pentafluorobenzene	
C_6HF_5O	771-61-9	61-034 /B+S1	Pentafluorophenol	
$C_6H_2F_4$	551-62-2	21-013	1,2,3,4-Tetrafluorobenzene	
	2367-82-0	21-014	1,2,3,5-Tetrafluorobenzene	
	327-54-8	21-015	1,2,4,5-Tetrafluorobenzene	
$C_6H_2F_5N$	771-60-8	64-014	2,3,4,5,6-Pentafluorobenzenamine	Pentafluoroaniline
$C_6H_3Cl_3$	87-61-6	22-056 /S1	1,2,3-Trichlorobenzene	
	120-82-1	22-035 /B+S1+S2	1,2,4-Trichlorobenzene	
	108-70-3	22-057 /S1	1,3,5-Trichlorobenzene	
$C_6H_3Cl_4N$	1929-82-4	64-015	2-Chloro-6-(trichloromethyl)pyridine	
C_6H_4BrCl	694-80-4	25-031	1-Bromo-2-chlorobenzene	*o*-Bromochlorobenzene
	108-37-2	25-032	1-Bromo-3-chlorobenzene	*m*-Bromochlorobenzene
	106-39-8	25-033 /B+S1	1-Bromo-4-chlorobenzene	*p*-Bromochlorobenzene
C_6H_4BrI	583-55-1	25-034	1-Bromo-2-iodobenzene	*o*-Bromoiodobenzene
	591-18-4	25-035	1-Bromo-3-iodobenzene	*m*-Bromoiodobenzene
	589-87-7	25-051 /S2	1-Bromo-4-iodobenzene	*p*-Iodobromobenzene; 4-Bromophenyl iodide
$C_6H_4BrNO_2$	585-79-5	64-016	1-Bromo-3-nitrobenzene	*m*-Bromonitrobenzene
$C_6H_4Br_2$	583-53-9	23-031	1,2-Dibromobenzene	*o*-Dibromobenzene
	108-36-1	23-032	1,3-Dibromobenzene	*m*-Dibromobenzene
	106-37-6	23-042 /S1	1,4-Dibromobenzene	*p*-Dibromobenzene
$C_6H_4Br_2O$	615-58-7	61-035	2,4-Dibromophenol	
C_6H_4ClI	637-87-6	25-049 /S1	1-Chloro-4-iodobenzene	*p*-Chloroiodobenzene
$C_6H_4ClNO_2$	88-73-3	64-042 /S2	1-Chloro-2-nitrobenzene	*o*-Nitrochlorobenzene

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	121-73-3	64-017 /B+S1+S2	1-Chloro-3-nitrobenzene	*m*-Chloronitrobenzene
	100-00-5	64-018 /B+S1	1-Chloro-4-nitrobenzene	*p*-Chloronitrobenzene
$C_6H_4Cl_2$	95-50-1	22-036 /B+S1+S2	1,2-Dichlorobenzene	*o*-Dichlorobenzene
	541-73-1	22-037 /B+S1+S2	1,3-Dichlorobenzene	*m*-Dichlorobenzene
	106-46-7	22-038 /B+S1	1,4-Dichlorobenzene	*p*-Dichlorobenzene
$C_6H_4F_2$	367-11-3	21-016 /B+S1	1,2-Difluorobenzene	*o*-Difluorobenzene
	372-18-9	21-017 /B+S1	1,3-Difluorobenzene	*m*-Difluorobenzene
	540-36-3	21-018 /B+S1	1,4-Difluorobenzene	*p*-Difluorobenzene
$C_6H_4I_2$	615-42-9	24-007	1,2-Di-iodobenzene	*o*-Diiodobenzene
	626-00-6	24-008	1,3-Di-iodobenzene	*m*-Di-iodobenzene
	624-38-4	24-017 /S2	1,4-Di-iodobenzene	*p*-Di-iodobenzene
$C_6H_4N_2O_4$	528-29-0	62-042	1,2-Dinitrobenzene	*o*-Di-nitrobenzene
	99-65-0	62-043	1,3-Dinitrobenzene	*m*-Di-nitrobenzene
	100-25-4	62-044	1,4-Dinitrobenzene	*p*-Di-nitrobenzene
$C_6H_4O_2$	106-51-4	43-015	2,5-Cyclohexadiene-1,4-dione	*p*-Benzoquinone; *p*-Quinone
C_6H_5Br	108-86-1	23-033 /B+S1	Bromobenzene	Phenyl bromide
C_6H_5BrO	106-41-2	61-036	4-Bromophenol	*p*-Bromophenol
C_6H_5Cl	108-90-7	22-039 /B+S1+S2	Chlorobenzene	Phenyl chloride
C_6H_5ClO	95-57-8	61-037/B+S1+S2	2-Chlorophenol	*o*-Chlorophenol
	108-43-0	61-051 /S1+S2	3-Chlorophenol	*m*-Chlorophenol
	106-48-9	61-052 /S1+S2	4-Chlorophenol	*p*-Chlorophenol
$C_6H_5Cl_3Si$	98-13-5	71-011	Trichlorophenylsilane	
C_6H_5F	462-06-6	21-019	Fluorobenzene	
C_6H_5FO	367-12-4	61-053 /S1	2-Fluorophenol	*o*-Fluorophenol
	372-20-3	61-054 /S1	3-Fluorophenol	*m*-Fluorophenol
	371-41-5	61-038	4-Fluorophenol	*p*-Fluorophenol
C_6H_5I	591-50-4	24-009 /B+S1	Iodobenzene	
$C_6H_5NO_2$	98-95-3	62-045 /B+S1	Nitrobenzene	
$C_6H_5NO_3$	88-75-5	62-046 /B+S1	2-Nitrophenol	*o*-Nitrophenol
	554-84-7	62-047	3-Nitrophenol	*m*-Nitrophenol
	100-02-7	62-048	4-Nitrophenol	*p*-Nitrophenol
C_6H_6	71-43-2	14-003/B+S1+S2	Benzene	
C_6H_6ClN	95-51-2	64-043 /S2	2-Chlorobenzenamine	2-Chloroaniline
	108-42-9	64-019	3-Chlorobenzenamine	*m*-Chloroaniline
	106-47-8	64-035 /S1	4-Chlorobenzenamine	4-Chlorophenylamine; *p*-Chloroaniline
C_6H_6FN	348-54-9	64-036 /S1	2-Fluorobenzenamine	*o*-Fluoroaniline
	371-40-4	64-020	4-Fluorobenzenamine	*p*-Fluoroaniline
$C_6H_6N_2O_2$	88-74-4	62-049	2-Nitrobenzenamine	*o*-Nitroaniline
	99-09-2	62-050	3-Nitrobenzenamine	*m*-Nitroaniline
	100-01-6	62-051	4-Nitrobenzenamine	*p*-Nitroaniline
C_6H_6O	108-95-2	42-034	Phenol	
$C_6H_6O_2$	120-80-9	42-035	1,2-Benzenediol	1,2-Dihydroxybenzene; Pyrocatechol; Catechol
	108-46-3	42-036	1,3-Benzenediol	1,3-Dihydroxybenzene; Resorcinol
	123-31-9	42-037	1,4-Benzenediol	1,4-Dihydroxybenzene; Hydroquinone
C_6H_6S	108-98-5	52-014	Benzenethiol	Thiophenol; Phenyl mercaptan
C_6H_7N	62-53-3	31-020 /B+S2	Benzenamine	Aniline; Aminobenzene; Phenylamine
	31357-71-8	32-017	Bicyclo[2.1.0]pentane-1-carbonitrile	1-Bicyclo[2.1.0]pentyl cyanide; 1-Cyanobicyclo[2.1.0]pentane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	15760-35-7	32-018	3-Methylenecyclobutanecarbonitrile	3-Methylenecyclobutyl cyanide; 1-Cyano-3-methylenecyclobutane
	109-06-8	33-013 /B+S1	2-Methylpyridine	β-Picoline
	108-99-6	33-014 /B+S1	3-Methylpyridine	β-Picoline
	108-89-4	33-015/B+S1	4-Methylpyridine	γ-Picoline
$C_6H_7NO_2$	7085-85-0	62-178 /S2	Ethyl ester 2-cyano-2-propenoic acid	Ethyl α-cyanoacrylate
C_6H_8	592-57-4	14-004	1,3-Cyclohexadiene	
	628-41-1	14-005	1,4-Cyclohexadiene	
$C_6H_8N_2$	108-45-2	31-021	1,3-Benzenediamine	1,3-Phenylenediamine
	100-63-0	34-007	Phenylhydrazine	
$C_6H_8N_2O_2$	4538-37-8	62-179 /S2	1,4-Diisocyanatobutane	Tetramethylene diisocyanate
C_6H_8O	930-68-7	43-065 /S1	2-Cyclohexen-1-one	
	625-86-5	46-028 /S1	2,5-Dimethylfuran	
$C_6H_8O_2$	637-88-7	43-016	1,4-Cyclohexanedione	Tetrahydroquinone
	4935-01-7	45-020	Methyl bicyclo[1.1.0]butane-1-carboxylate	Methyl ester bicyclo[1.1.0]butane-1-carboxylic acid
$C_6H_8O_4$	624-48-6	45-021	Dimethyl (*Z*)-2-butenedioate	Dimethyl ester (*Z*)-2-butenedioic acid; Dimethyl *cis*-2-butenedioate; Dimethyl maleate
	95-96-5	47-018	3,6-Dimethyl-1,4-dioxane-2,5-dione	
	4511-42-6	47-056 /S1	(3*S*,6*S*)-3,6-Dimethyl-1,4-dioxane-2,5-dione	*l*-Lactide
C_6H_8S	638-02-8	53-011	2,5-Dimethylthiophene	
C_6H_9N	4254-02-8	32-019	Cyclopentanecarbonitrile	Cyclopentyl cyanide; Cyanocyclopentane
	625-82-1	33-016 /B+S1	2,4-Dimethyl-1*H*-pyrrole	
	625-84-3	33-017	2,5-Dimethyl-1*H*-pyrrole	
C_6H_9NO	88-12-0	62-146 /S1	1-Ethenyl-2-pyrrolidinone	*N*-Vinylpyrrolidone
$C_6H_9NO_2$	1572-99-2	62-147 /S1	Ethyl ester 2-cyanopropanoic acid	Ethyl ester cyanomethylacetic acid
C_6H_{10}	110-83-8	14-006 /B+S1	Cyclohexene	1,2,3,4-Tetrahydrobenzene
	592-42-7	13-025	1,5-Hexadiene	Diallyl
	693-89-0	14-007	1-Methylcyclopentene	
	1120-62-3	14-008	3-Methylcyclopentene	
$C_6H_{10}O$	108-94-1	43-017 /B+S1+S2	Cyclohexanone	Pimelic ketone; Ketohexamethylene
	109-49-9	43-073 /S2	5-Hexen-2-one	5-Oxo-1-hexene; Allylacetone
	141-79-7	43-018 /B+S1	4-Methyl-3-penten-2-one	Mesityl oxide
	286-20-4	46-017	7-Oxabicyclo[4.1.0]heptane	1,2-Epoxycyclohexane; Cyclohexene oxide
$C_6H_{10}O_2$	4606-07-9	45-022	Ethyl cyclopropanecarboxylate	Ethyl ester cyclopropanecarboxylic acid
	765-85-5	45-023	Methyl cyclobutanecarboxylate	Methyl ester cyclobutanecarboxylic acid
	502-44-3	47-019	2-Oxepanone	ε-Caprolactone; 6-Hexanolide
	2408-20-0	45-024	2-Propenyl propanoate	Allyl propionate
$C_6H_{10}O_3$	141-97-9	47-020 /B+S1	Ethyl ester 3-oxobutanoic acid	Ethyl 3-oxobutanoate; Ethyl acetoacetate; Ethyl ester acetoacetic acid
$C_6H_{10}O_4$	95-92-1	45-025	Diethyl ethanedioate	Diethyl ester ethanedioic acid; Diethyl oxalate
	609-02-9	45-133 /S1	Dimethyl ester methylpropanedioic acid	Dimethyl methylmalonate
	111-55-7	45-026 /B+S1	1,2-Ethanediol diacetate	1,2-Ethanediyl ester acetic acid; Ethylene glycol diacetate
	124-04-9	44-013	Hexanedioic acid	Adipic acid; 1,4-Butanedicarboxylic acid
$C_6H_{11}BF_4N_2$	143314-16-3	75-001 /S1+S2	1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_6H_{11}Br$	108-85-0	23-043 /S1	Bromocyclohexane	Cyclohexyl bromide
$C_6H_{11}Cl$	542-18-7	22-058 /S1	Chlorocyclohexane	Cyclohexyl chloride
	6196-85-6	22-059 /S1	1-Chloro-1-methylcyclopentane	
$C_6H_{11}F_6N_2P$	155371-19-0	75-002 /S2	1-Ethyl-3-methyl-1*H*-imidazolium hexafluorophosphate	[Emim][PF6]; [C2mim][PF6]
$C_6H_{11}KO_2$	19455-00-6	74-032/S2	Potassium salt hexanoic acid	Potassium hexanoate; Potassium caproate
$C_6H_{11}N$	628-73-9	32-020	Hexanenitrile	Capronitrile; Amyl cyanide
$C_6H_{11}NO$	100-64-1	62-052 /B+S2	Cyclohexanone oxime	
	2687-91-4	62-180 /S2	1-Ethyl-2-pyrrolidinone	*N*-Ethyl-2-pyrrolidinone; *N*-Ethylbutyrolactam
	105-60-2	62-053 /B+S2	Hexahydro-2*H*-azepin-2-one	ε-Caprolactam; 6-Hexanelactam; 6-Aminohexanoic lactam
$C_6H_{11}NO_2$	14618-78-1	62-054	4,4-Dimethoxybutanenitrile	β-Cyanopropionaldehyde dimethyl acetal
	54953-79-6	62-148 /S1	Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one	5,5-Dimethylperhydro-1,3-oxazin-2-one
C_6H_{12}	110-82-7	12-007 /B+S1+S2	Cyclohexane	Hexamethylene
	563-79-1	13-026	2,3-Dimethyl-2-butene	Tetramethylethylene
	558-37-2	13-027	3,3-Dimethyl-1-butene	*tert*-Butylethylene; Neohexene
	592-41-6	13-028	1-Hexene	Hexylene
	7688-21-3	13-029	(*Z*)-2-Hexene	*cis*-2-Hexene
	96-37-7	12-008	Methylcyclopentane	
	691-37-2	13-040 /S1	4-Methyl-1-pentene	
$C_6H_{12}BNO_3$	283-56-7	72-007	2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3] undecane	2,2′,2″-Nitrilotriethanol cyclic ester with boric acid (1:1); Triethanolamine borate
$C_6H_{12}Br_2$	629-03-8	23-045 /S2	1,6-Dibromohexane	Hexamethylene dibromide
$C_6H_{12}Cl_2$	2163-00-0	22-040 /B+S2	1,6-Dichlorohexane	Hexamethylene chloride
$C_6H_{12}Cl_3O_4P$	115-96-8	72-008	2-Chloroethanol phosphate (3:1)	Tri(2-chloroethyl)phosphate
$C_6H_{12}N_2$	280-57-9	33-018	1,4-Diazobicyclo[2.2.2]octane	Triethylenediamine
	627-70-3	34-008	(1-Methylethylidene)hydrazone 2-propanone	Acetone azine; Dimethyl ketazine
$C_6H_{12}O$	108-93-0	42-038 /B+S1	Cyclohexanol	Cyclohexyl alcohol; Hexahydrophenol
	75-97-8	43-019	3,3-Dimethyl-2-butanone	*tert*-Butyl methyl ketone; Pinacolone
	111-34-2	41-013 /B+S1	1-(Ethenyloxy)butane	Butyl vinyl ether; Butoxyethylene
	109-53-5	41-014	1-(Ethenyloxy)-2-methylpropane	Isobutyl vinyl ether; Isobutoxyethylene
	66-25-1	43-020	Hexanal	Hexaldehyde; Caproaldehyde
	591-78-6	43-021	2-Hexanone	Butyl methyl ketone
	589-38-8	43-022	3-Hexanone	Ethyl propyl ketone
	1462-03-9	42-110 /S1+S2	1-Methylcyclopentanol	
	108-10-1	43-023	4-Methyl-2-pentanone	Isobutyl methyl ketone
$C_6H_{12}O_2$	123-86-4	45-027 /B+S1	Butyl acetate	Butyl ethanoate
	595-37-9	44-042 /S2	2,2-Dimethylbutanoic acid	2,2-Dimethylbutyric acid; Neohexanoic acid
	540-88-5	45-028	1,1-Dimethylethyl acetate	1,1-Dimethylethyl ethanoate; *tert*-Butyl acetate
	105-54-4	45-029	Ethyl butanoate	Ethyl butyrate
	97-62-1	45-030	Ethyl 2-methylpropanoate	Ethyl isobutyrate
	142-62-1	44-014	Hexanoic acid	Caproic acid

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	110-45-2	45-033	3-Methylbutyl formate	3-Methylbutyl methanoate; Isoamyl formate; Isopentyl formate
	598-98-1	45-031	Methyl 2,2-dimethylpropanoate	Methyl ester 2,2-dimethylpropanoic acid; Methyl pivalate; Methyl trimethylacetate
	624-24-8	45-032	Methyl pentanoate	Methyl valerate
	110-19-0	45-034	2-Methylpropyl acetate	2-Methylpropyl ethanoate; Isobutyl acetate
	106-36-5	45-035 /B+S1	Propyl propanoate	Propyl propionate
	100-72-1	47-021	Tetrahydro-2*H*-pyran-2-methanol	
$C_6H_{12}O_3$	111-15-9	47-022 /B+S1	2-Ethoxyethanol acetate	2-Ethoxyethyl acetate; Cellosolve acetate
	123-63-7	46-018	2,4,6-Trimethyl-1,3,5-trioxane	Paraldehyde
$C_6H_{12}S$	1569-69-3	52-015	Cyclohexanethiol	Cyclohexyl mercaptan
	7133-36-0	51-013	Methylthiocyclopentane	Cyclopentyl methyl sulfide
$C_6H_{12}Si$	6224-91-5	71-062 /S1	Trimethyl-1-propynylsilane	1-Trimethylsilyl-1-propyne
$C_6H_{13}Br$	111-25-1	23-034 /B+S1+S2	1-Bromohexane	*n*-Hexyl bromide
	3377-87-5	23-035	3-Bromohexane	
$C_6H_{13}Cl$	544-10-5	22-060 /S1+S2	1-Chlorohexane	*n*-Hexyl chloride
$C_6H_{13}I$	638-45-9	24-015 /S1+S2	1-Iodohexane	*n*-Hexyl iodide
$C_6H_{13}N$	108-91-8	31-022 /B+S2	Cyclohexanamine	Cyclohexylamine
	111-49-9	33-019	Hexahydro-1*H*-azepine	Perhydroazepine; Hexamethylenimine; Azacycloheptane
	626-67-5	33-020	1-Methylpiperidine	*N*-Methylpiperidine
	109-05-7	33-021	2-Methylpiperidine	2-Pipecoline; α-Pipecoline
	626-58-4	33-022	4-Methylpiperidine	4-Pipecoline; γ-Pipecoline
$C_6H_{13}NO$	1119-49-9	62-055	*N*-Butylacetamide	*N*-Butylethanamide
	685-91-6	62-056	*N*,*N*-Diethylacetamide	*N*,*N*-Diethylethanamide
	6225-10-1	62-057	*N*-Methylpentanamide	*N*-Methylvaleramide
$C_6H_{13}NO_2$	33229-89-9	62-149 /S1	Ethyl ester *N*,*N*-dimethylglycine	Ethyl ester *N*,*N*-dimethylaminoacetic acid
	42293-86-7	62-150 /S1	Methyl ester *N*,*N*-dimethyl-*L*-alanine	Methyl ester 2-dimethylaminopropionic acid
C_6H_{14}	75-83-2	11-011	2,2-Dimethylbutane	Neohexane
	79-29-8	11-012	2,3-Dimethylbutane	Diisopropyl
	110-54-3	11-013 /B+S1+S2	Hexane	
	107-83-5	11-014	2-Methylpentane	Dimethylpropylmethane
	96-14-0	11-015	3-Methylpentane	Diethylmethylmethane
$C_6H_{14}N_2O$	17697-55-1	62-058	Dipropyldiazene 1-oxide	
$C_6H_{14}O$	624-95-3	42-039 /B+S1+S2	3,3-Dimethyl-1-butanol	
	637-92-3	41-015 /B+S2	2-Ethoxy-2-methylpropane	*tert*-Butyl ethyl ether
	97-95-0	42-040	2-Ethyl-1-butanol	2-Ethylbutyl alcohol
	111-27-3	42-041 /B+S1+S2	1-Hexanol	Hexyl alcohol
	626-93-7	42-042	2-Hexanol	
	623-37-0	42-043	3-Hexanol	Ethyl propyl carbinol
	994-05-8	41-016 /B+S2	2-Methoxy-2-methylbutane	Methyl *tert*-pentyl ether; 3,3-Dimethyl-2-oxapentane; *tert*-Amyl methyl ether
	105-30-6	42-044	2-Methyl-1-pentanol	
	590-36-3	42-045	2-Methyl-2-pentanol	
	565-60-6	42-046	3-Methyl-2-pentanol	
	77-74-7	42-047 /B+S2	3-Methyl-3-pentanol	
	108-11-2	42-048	4-Methyl-2-pentanol	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	111-43-3	41-017 /B+S1	1,1′-Oxybis(propane)	Dipropyl ether
	108-20-3	41-018 /B+S1+S2	2,2′-Oxybis(propane)	1,1′-Bis(methylethyl) ether; Diisopropyl ether
$C_6H_{14}O_2$	111-76-2	47-023 /B+S1+S2	2-Butoxyethanol	3-Oxa-1-heptanol; Ethylene glycol monobutyl ether; Butyl cellosolve
	105-57-7	41-019	1,1-Diethoxyethane	Acetaldehyde diethyl acetal; Acetal
	629-14-1	41-020	1,2-Diethoxyethane	3,6-Dioxaoctane; Ethylene glycol diethyl ether; Diethyl cellosolve
	7580-85-0	47-079 /S2	2-(1,1-Dimethylethoxy)ethanol	2-*tert*-Butoxyethanol; Ethylene glycol *tert*-butyl ether
	629-11-8	42-111 /S1+S2	1,6-Hexanediol	
	17081-22-0	41-021	1-Methoxy-2-propoxyethane	2,5-Dioxaoctane; Ethylene glycol methyl ether propyl ether
	4439-24-1	47-057 /S1	2-(2-Methylpropoxy)ethanol	2-Isobutoxyethanol
$C_6H_{14}O_3$	111-90-0	47-024 /B+S1	2-(2-Ethoxyethoxy)ethanol	Diethylene glycol monoethyl ether
	77-99-6	42-049	2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	1,1,1-Tris(hydroxymethyl)propane; Trimethylolpropane
	106-62-7	47-058 /S1	2-(2-Hydroxypropoxy)-1-propanol	Di(propylene glycol)
	111-96-6	41-022 /B+S1	1,1′-Oxybis(2-methoxyethane)	2,5,8-Trioxanonane; Diethylene glycol dimethyl ether; Diglyme
$C_6H_{14}O_4$	112-27-6	47-025 /B+S1+S2	2,2′-[1,2-Ethanediylbis(oxy)]bis(ethanol)	1,8-Dihydroxy-3,6-dioxaoctane; Triethylene glycol
$C_6H_{14}O_6$	69-65-8	42-050	*D*-Mannitol	
$C_6H_{14}S$	111-31-9	52-016 /B+S1	1-Hexanethiol	1-Hexyl mercaptan
	13286-91-4	51-014	2-(Methylthio)pentane	3-Methyl-2-thiahexane; Methyl 1-methylbutyl sulfide
	111-47-7	51-015	1,1′-Thiobis(propane)	Dipropyl sulfide
	625-80-9	51-016	2,2′-Thiobis(propane)	Bis(1-methylethyl) sulfide; Diisopropyl sulfide
$C_6H_{14}S_2$	629-19-6	51-017	Dipropyl disulfide	4,5-Dithiaoctane
$C_6H_{15}Al$	97-93-8	73-018	Triethylaluminum	
$C_6H_{15}As$	617-75-4	73-019	Triethylarsine	
$C_6H_{15}B$	97-94-9	72-009	Triethylborane	
$C_6H_{15}Bi$	617-77-6	73-020	Triethylbis(muthine)	
$C_6H_{15}ClSi$	994-30-9	71-012	Chlorotriethylsilane	
$C_6H_{15}Ga$	1115-99-7	73-021	Triethylgallium	
$C_6H_{15}In$	923-34-2	73-022	Triethylindium	
$C_6H_{15}N$	121-44-8	31-023 /B+S1+S2	*N*,*N*-Diethylethanamine	Triethylamine
	111-26-2	31-024 /B+S1+S2	1-Hexanamine	Hexylamine
	108-18-9	31-047 /S1	*N*–(1-Methylethyl)-2-propanamine	Diisopropylamine
	142-84-7	31-025 /B+S1+S2	*N*-Propyl-1-propanamine	Dipropylamine
$C_6H_{15}NO$	100-37-8	62-151 /S1+S2	2-(Diethylamino)ethanol	Diethylethanolamine
$C_6H_{15}NO_2$	139-87-7	62-152 /S1	2,2′-(Ethylimino)bis(ethanol)	Ethyldiethanolamine; 2-[Ethyl(2-hydroxyethyl) amino]ethanol
	110-97-4	62-153 /S1	1,1′-Iminobis(2-propanol)	Di-2-propanolamine; Bis(2-hydroxypropyl)amine; 1,1′-Azanediylbis(propan-2-ol)
$C_6H_{15}NO_3$	102-71-6	62-059 /B+S1	2,2′,2″-Nitrilotris(ethanol)	Tri(2-hydroxyethyl)amine; Triethanolamine
$C_6H_{15}N_3$	140-31-8	33-023	1-Piperazineethanamine	*N*–(2-Aminoethyl)piperazine
$C_6H_{15}P$	554-70-1	72-017 /S1	Triethylphosphine	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_6H_{15}Sb$	617-85-6	73-023	Triethylstibine	Triethylantimony
$C_6H_{16}N_2O_2$	4439-20-7	62-154 /S1	2,2′-(1,2-Ethanediyldiimino)bis(ethanol)	2,2′-(Ethylenediimino)diethanol; *N*,*N*′-Bis(2-hydroxyethyl) ethylenediamine
$C_6H_{16}Si_2$	1627-98-1	71-013	1,1,3,3-Tetramethyl-1,3-disilacyclobutane	
$C_6H_{18}AsN_3$	6596-96-9	73-055 /S2	Hexamethylarsenous triamide	Tris(dimethylamino)arsine
$C_6H_{18}BN$	1722-26-5	72-010	Triethylamineborane	*N*,*N*-Dimethylethanamine compd. with borane (1:1)
$C_6H_{18}N_3OP$	680-31-9	72-011 /B+S1	Hexamethyl phosphoric triamide	Hexamethylphosphoramide
$C_6H_{18}N_3P$	1608-26-0	72-023 /S2	Hexamethylphosphorous triamide	Tris(dimethylamino-phosphorus); Hexametapil
$C_6H_{18}N_4$	112-24-3	31-026	*N*,*N*′-Bis(2-aminoethyl)-1,2-ethanediamine	Triethylenetetramine
$C_6H_{18}OSi_2$	107-46-0	71-014	Hexamethyldisiloxane	
$C_6H_{18}O_3Si_3$	541-05-9	71-015 /B+S2	Hexamethylcyclotrisiloxane	
$C_6H_{18}Si_2$	1450-14-2	71-016	Hexamethyldisilane	
$C_6H_{21}N_3Si_3$	1009-93-4	71-017	2,2,4,4,6,6-Hexamethylcyclotrisilazane	Dimethylaminosilane trimer
C_7F_8	434-64-0	21-020	Pentafluoro(trifluoromethyl)benzene	Octafluorotoluene; Perfluorotoluene
C_7F_{14}	355-02-2	21-021	(Trifluoromethyl)undecafluorocyclohexane	Perfluoromethylcyclohexane
C_7F_{16}	335-57-9	21-022 /B+S1	Hexadecafluoroheptane	Perfluoroheptane
$C_7HF_{13}O_2$	375-85-9	61-058 /S2	Tridecafluoroheptanoic acid	Perfluoroenanthic acid
$C_7H_3F_5$	771-56-2	21-023	Pentafluoromethylbenzene	2,3,4,5,6-Pentafluorotoluene
C_7H_4ClNO	2909-38-8	64-021	1-Chloro-3-isocyanatobenzene	*m*-Chlorophenylisocyanate
$C_7H_4Cl_2O$	874-42-0	61-059 /S2	2,4-Dichlorobenzaldehyde	*o*,*p*-Dichlorobenzaldehyde
$C_7H_4F_3NO_2$	98-46-4	64-022	1-Nitro-3-(trifluoromethyl)benzene	*m*-Trifluoromethylnitrobenzene
$C_7H_4N_2O_5$	528-75-6	62-181 /S2	2,4-Dinitrobenzaldehyde	
C_7H_5ClO	98-88-4	61-039	Benzoyl chloride	
$C_7H_5ClO_2$	118-91-2	61-040	2-Chlorobenzoic acid	*o*-Chlorobenzoic acid
	535-80-8	61-041	3-Chlorobenzoic acid	*m*-Chlorobenzoic acid
	74-11-3	61-042 /B+S2	4-Chlorobenzoic acid	*p*-Chlorobenzoic acid
$C_7H_5F_3$	98-08-8	21-024	(Trifluoromethyl)benzene	α,α,α-Trifluorotoluene
$C_7H_5F_4NO_2$	27827-91-4	64-037 /S1	2,2,3,3-Tetrafluoropropyl ester 2-cyano-2-propenic acid	1,1,2,2-Tetrafluoropro-3-yl 2-cyanoacrylate; 1,1,3-Trihydrotetrafluoropropyl α-cyanoacrylate
C_7H_5N	100-47-0	32-021 /B+S1+S2	Benzonitrile	Phenyl cyanide
C_7H_5NO	273-53-0	62-060	Benzoxazole	
	103-71-9	62-155 /S1	Isocyanatobenzene	Phenyl isocyanate
$C_7H_5NO_4$	552-16-9	62-061	2-Nitrobenzoic acid	*o*-Nitrobenzoic acid; *o*-Nitrodracylic acid
	121-92-6	62-062	3-Nitrobenzoic acid	*m*-Nitrobenzoic acid; *m*-Nitrodracylic acid
	62-23-7	62-063	4-Nitrobenzoic acid	*p*-Nitrobenzoic acid; *p*-Nitrodracylic acid
C_7H_5NS	95-16-9	64-023	Benzothiazole	
	103-72-0	64-024	Isothiocyanatobenzene	Phenyl ester isothiocyanic acid
$C_7H_5N_3O_6$	118-96-7	62-064	2-Methyl-1,3,5-trinitrobenzene	2,4,6-Trinitrotoluene; Tritol; TNT
$C_7H_5N_5O_8$	479-45-8	62-065	*N*-Methyl-*N*,2,4,6-tetranitrobenzeneamine	Trinitrophenylmethylnitroamine; Tetryl
$C_7H_6F_8O_3$	1422-70-4	61-043	Bis(2,2,3,3-tetrafluoropropyl) ester carbonic acid	Bis(2,2,3,3-tetrafluoropropyl) carbonate
$C_7H_6N_2O_4$	606-20-2	62-066	2-Methyl-1,3-dinitrobenzene	2,6-Dinitrotoluene
C_7H_6O	100-52-7	43-024	Benzaldehyde	Benzoic aldehyde

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_7H_6O_2$	65-85-0	44-015	Benzoic acid	Benzenecarboxylic acid; Carboxybenzene; Phenylformic acid
	90-02-8	47-026	2-Hydroxybenzaldehyde	Salicyl aldehyde
$C_7H_6O_3$	69-72-7	47-027	2-Hydroxybenzoic acid	Salicylic acid
C_7H_7Br	106-38-7	23-046 /S2	1-Bromo-4-methylbenzene	*p*-Bromotoluene; 4-Tolyl bromide
C_7H_7Cl	100-44-7	22-041	(Chloromethyl)benzene	Benzyl chloride
	95-49-8	22-042	1-Chloro-2-methylbenzene	2-Chlorotoluene; *o*-Chlorotoluene; *o*-Tolyl chloride
	106-43-4	22-065 /S2	1-Chloro-4-methylbenzene	*p*-Chlorotoluene; 4-Tolylchloride
C_7H_7F	95-52-3	21-025	1-Fluoro-2-methylbenzene	2-Fluorotoluene; *o*-Tolyl fluoride
	352-70-5	21-026	1-Fluoro-3-methylbenzene	3-Fluorotoluene; *m*-Tolyl fluoride
	352-32-9	21-027	1-Fluoro-4-methylbenzene	*p*-Fluorotoluene; *p*-Tolyl fluoride
C_7H_7I	624-31-7	24-018 /S2	1-Iodo-4-methylbenzene	*p*-Iodotoluene; 4-Tolyl iodide
C_7H_7NO	55-21-0	62-067	Benzamide	
$C_7H_7NO_2$	99-08-1	62-068	1-Methyl-3-nitrobenzene	*m*-Nitrotoluene
	99-99-0	62-069	1-Methyl-4-nitrobenzene	*p*-Nitrotoluene
	7324-02-9	62-156 /S1	2-Propenyl ester 2-cyano-2-propenoic acid	Allyl α-cyanoacrylate
$C_7H_7NO_3$	91-23-6	62-070	1-Methoxy-2-nitrobenzene	*o*-Nitroanisole
	555-03-3	62-071	1-Methoxy-3-nitrobenzene	*m*-Nitroanisole
	100-17-4	62-072	1-Methoxy-4-nitrobenzene	*p*-Nitroanisole
C_7H_8	121-46-0	14-009 /B+S1+S2	Bicyclo[2.2.1]hepta-2,5-diene	2,5-Norbornadiene
	544-25-2	14-010	1,3,5-Cycloheptatriene	
	108-88-3	14-011 /B+S1+S2	Methylbenzene	Toluene; Phenyl methane
	278-06-8	12-009 /B+S1	Tetracyclo[3.2.0.$0^{2,7}$.$0^{4,6}$]heptane	Quadricyclane
$C_7H_8Cl_2Si$	149-74-6	71-018	Dichloromethylphenylsilane	
C_7H_8O	100-51-6	42-051 /B+S2	Benzenemethanol	Benzyl alcohol
	100-66-3	41-023	Methoxybenzene	Methyl phenyl ether; Anisole
	95-48-7	42-052	2-Methylphenol	*o*-Hydroxytoluene; *o*-Cresol
	108-39-4	42-053	3-Methylphenol	*m*-Hydroxytoluene; *m*-Cresol
	106-44-5	42-054	4-Methylphenol	*p*-Hydroxytoluene; *p*-Cresol
$C_7H_8O_2$	1004-36-0	47-028	2,6-Dimethyl-4*H*-pyran-4-one	2,6-Dimethyl-γ-pyrone
C_7H_8S	100-68-5	51-018	Methylthiobenzene	Methyl phenyl sulfide
$C_7H_9Cl_3OS$	79886-21-8	64-038 /S1	*O*-Butyl ester 2,3,3-trichloro-2-propenethioic acid	*O*-Butyl ester trichlorothioacrylic acid; *n*-Butyl ester trichlorothioacrylate
C_7H_9N	100-46-9	31-027	Benzenemethanamine	Benzylamine; Phenylmethylamine; Aminotoluene
	31357-72-9	32-022	Bicyclo[3.1.0]hexane-1-carbonitrile	1-Bicyclo[3.1.0]hexyl cyanide; 1-Cyanobicyclo[3.1.0]hexane
	583-61-9	33-024 /B+S1	2,3-Dimethylpyridine	2,3-Lutidine
	108-47-4	33-025 /B+S1	2,4-Dimethylpyridine	2,4-Lutidine
	589-93-5	33-026 /B+S1	2,5-Dimethylpyridine	2,5-Lutidine
	108-48-5	33-027 /B+S1	2,6-Dimethylpyridine	2,6-Lutidine
	583-58-4	33-028 /B+S1	3,4-Dimethylpyridine	3,4-Lutidine
	591-22-0	33-029 /B+S1	3,5-Dimethylpyridine	3,5-Lutidine

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	100-61-8	31-028	*N*-Methylbenzenamine	*N*-Methylaniline; Methylphenylamine
	95-53-4	31-029 /B+S1	2-Methylbenzenamine	2-Methylaniline; *o*-Toluidine
	108-44-1	31-030 /B+S1	3-Methylbenzenamine	3-Methylaniline; *m*-Toluidine
	106-49-0	31-031 /B+S1	4-Methylbenzenamine	4-Methylaniline; *p*-Toluidine
C_7H_{10}	498-66-8	14-099 /S1	Bicyclo[2.2.1]hept-2-ene	Norbornene; Norbornylene
$C_7H_{10}ClN_3O_3$	16773-42-5	64-044 /S2	α-(Chloromethyl)-2-methyl-5-nitro-1*H*-imidazole-1-ethanol	Ornidazole
$C_7H_{11}F_3N_2O_3S$	145022-44-2	75-003 /S2	1-Ethyl-3-methylimidazolium trifluoromethansulfonate	1-Ethyl-3-methylimidazolium trifluoromethanesulfonic acid
$C_7H_{11}N$	766-05-2	32-023	Cyclohexanecarbonitrile	Cyclohexyl cyanide; Cyanocyclohexane
	931-53-3	32-027 /S1	Isocyanocyclohexane	
C_7H_{12}	286-08-8	12-010	Bicyclo[4.1.0]heptane	Norcarane
	45510-00-7	14-012	(*Z*)-Cycloheptene	*cis*-Cycloheptene
	2146-38-5	14-013	1-Ethylcyclopentene	
	2146-37-4	12-011	Ethylidenecyclopentane	
	591-47-9	14-014	4-Methylcyclohexene	
	1192-37-6	12-012	Methylenecyclohexane	
$C_7H_{12}O$	502-42-1	43-025	Cycloheptanone	Suberone
	583-60-8	43-026	2-Methylcyclohexanone	*o*-Methylcyclohexanone
	591-24-2	43-027	3-Methylcyclohexanone	*m*-Methylcyclohexanone
	589-92-4	43-028	4-Methylcyclohexanone	*p*-Methylcyclohexanone
$C_7H_{12}O_2$	141-32-2	45-036 /B+S1	Butyl 2-propenoate	Butyl ester 2-propenoic acid; Butyl acrylate
	4351-54-6	45-162 /S2	Cyclohexyl formate	Cyclohexyl ester formic acid
	2051-78-7	45-037	2-Propenyl butanoate	Allyl butyrate
	15727-77-2	45-038	2-Propenyl 2-methylpropanoate	2-Propenyl ester 2-methylpropanoic acid; Allyl isobutyrate
$C_7H_{12}O_4$	105-53-3	45-039 /B+S1	Diethyl propanedioate	Diethyl ester propanedioic acid; Diethyl malonate
	6065-54-9	45-134 /S1	Dimethyl ester dimethylpropanedioic acid	Dimethyl dimethylmalonate
	111-16-0	44-043 /S2	Heptanedioic acid	1,5-Pentanedicarboxylic acid; Pimelic acid; Pileric acid
$C_7H_{13}Cl$	931-78-2	22-061 /S1	1-Chloro-1-methylcyclohexane	
$C_7H_{13}NO$	673-66-5	62-073	Hexahydro-2(1*H*)-azocinone	ω-Enantholactam
	162047-91-8	62-157 /S1	2-Methoxy-3,3-dimethylbutanenitrile	
	162047-90-7	62-158 /S1	2-Methoxy-2-methylpentanenitrile	
C_7H_{14}	291-64-5	12-013	Cycloheptane	
	1638-26-2	12-014	1,1-Dimethylcyclopentane	
	1192-18-3	12-015	*cis*-1,2-Dimethylcyclopentane	
	822-50-4	12-016	*trans*-1,2-Dimethylcyclopentane	
	1759-58-6	12-017	*trans*-1,3-Dimethylcyclopentane	
	1640-89-7	12-018	Ethylcyclopentane	
	592-76-7	13-030 /B+S1	1-Heptene	1-Heptylene
	108-87-2	12-019 /B+S1+S2	Methylcyclohexane	Hexahydrotoluene
$C_7H_{14}ClNO$	27086-19-7	64-025	Dipropylcarbamic chloride	*N*,*N*-Dipropylcarbamoyl chloride
$C_7H_{14}O$	502-41-0	42-055	Cycloheptanol	
	19353-21-0	43-029	3,4-Dimethylpentanal	3,4-Dimethylvaleraldehyde
	565-80-0	43-030	2,4-Dimethyl-3-pentanone	Diisopropyl ketone
	111-71-7	43-031	Heptanal	Heptyl aldehyde; Enanthaldehyde

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	110-43-0	43-032 /B+S2	2-Heptanone	Methyl pentyl ketone
	123-19-3	43-033	4-Heptanone	Dipropyl ketone
	590-67-0	42-056 /B+S1	1-Methylcyclohexanol	
	7443-70-1	42-058	*cis*-2-Methylcyclohexanol	
	7443-52-9	42-059	*trans*-2-Methylcyclohexanol	
	591-23-1	42-060	3-Methylcyclohexanol	*m*-Methylcyclohexanol (unspec. isomer, chirality)
	589-91-3	42-061	4-Methylcyclohexanol	*p*-Methylcyclohexanol (unspeci. isomer)
	19269-28-4	43-034	3-Methylhexanal	
	7379-12-6	43-035	2-Methyl-3-hexanone	
$C_7H_{14}O_2$	3938-95-2	45-040 /B+S1+S2	Ethyl 2,2-dimethylpropanoate	Ethyl ester 2,2-dimethylpropanoic acid; Ethyl pivalate
	7452-79-1	45-135 /S1	Ethyl ester 2-methylbutanoic acid	Ethyl 2-methylbutyrate
	108-64-5	45-041	Ethyl 3-methylbutanoate	Ethyl isovalerate
	539-82-2	45-042	Ethyl pentanoate	Ethyl valerate
	111-14-8	44-016	Heptanoic acid	Enanthic acid
	123-92-2	45-043 /B+S2	3-Methylbutyl acetate	3-Methylbutyl ethanoate; Isoamyl acetate; Isopentyl acetate
	540-42-1	45-044	2-Methylpropyl propanoate	Isobutyl propionate
	628-63-7	45-045 /B+S1	Pentyl acetate	Pentyl ethanoate; Amyl acetate
	105-66-8	45-046 /B+S1	Propyl butanoate	Propyl butyrate
	644-49-5	45-047	Propyl 2-methylpropanoate	Propyl isobutyrate
$C_7H_{14}O_3$	20267-19-0	47-059 /S1	2-Hydroxyethyl ester 2,2-dimethylpropanoic acid	2-Hydroxyethyl pivalate
$C_7H_{14}Si$	2043-08-5	71-066 /S2	Methyldi-2-propenylsilane	Methyldiallylsilane
$C_7H_{15}Br$	629-04-9	23-036 /B+S1+S2	1-Bromoheptane	*n*-Heptyl bromide
$C_7H_{15}C$	629-06-1	22-062 /S1+S2	1-Chloroheptane	Heptyl chloride
	999-52-0	22-043	3-Chloroheptane	
$C_7H_{15}I$	4282-40-0	24-016 /S1+S2	1-Iodoheptane	Heptyl iodide
$C_7H_{15}N$	1121-92-2	33-030	Octahydroazocine	Perhydroazocine; Heptamethylenimine
$C_7H_{15}NO$	1484-84-0	62-159 /S1	2-Piperidineethanol	2-Piperidin-2-ylethanol
$C_7H_{15}NO_2$	140653-59-4	62-160 /S1	Methyl ester *N*,*N*,2-trimethylalanine	Methyl ester 2-dimethylamino-2-methylpropanoic acid
C_7H_{16}	590-35-2	11-016	2,2-Dimethylpentane	
	565-59-3	11-017	2,3-Dimethylpentane	
	108-08-7	11-018	2,4-Dimethylpentane	
	562-49-2	11-019	3,3-Dimethylpentane	
	617-78-7	11-020	3-Ethylpentane	Triethylmethane
	142-82-5	11-021	Heptane	Dipropylmethane
	591-76-4	11-022	2-Methylhexane	Isoheptane; Ethylisobutylmethane
	589-34-4	11-023	3-Methylhexane	
	464-06-2	11-024	2,2,3-Trimethylbutane	Isopropyltrimethylmethane; Triptane
$C_7H_{16}O$	919-94-8	41-024 /B+S2	2-Ethoxy-2-methylbutane	Ethyl *tert*-pentyl ether; 4,4-Dimethyl-3-oxahexane; *tert*-Amyl ethyl ether
	597-49-9	42-062 /B+S2	3-Ethyl-3-pentanol	
	111-70-6	42-063 /B+S1+S2	1-Heptanol	Heptyl alcohol
	543-49-7	42-064	2-Heptanol	
	589-55-9	42-065	4-Heptanol	Dipropyl carbinol
	17348-59-3	41-052 /S2	2-Methyl-2-(1-methylethoxy)propane	*tert*-Butyl isopropyl ether
	29072-93-3	41-053 /S2	2-Methyl-2-propoxypropane	*tert*-Butyl propyl ether
$C_7H_{16}O_2$	13343-98-1	41-025	1-Butoxy-2-methoxyethane	2,5-Dioxanonane; Ethylene glycol butyl ether methyl ether

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	3459-83-4	41-026	1,3-Diethoxypropane	3,7-Dioxanonane; Propylene glycol diethyl ether
	111-89-7	41-027	1,5-Dimethoxypentane	2,8-Dioxanonane; Pentylene glycol dimethyl ether
	36865-47-1	41-028	1-Ethoxy-4-methoxybutane	2,7-Dioxanonane; Butylene glycol ethyl ether methyl ether
	18854-31-4	41-029	1-Ethoxy-2-propoxyethane	3,6-Dioxanonane; Ethylene glycol ethyl ether propyl ether
	89851-49-0	41-030	1-Methoxy-3-propoxypropane	2,6-Dioxanonane; Propylene glycol methyl ether propyl ether
$C_7H_{16}O_3$	122-51-0	41-031	1,1′,1″-[Methylidynetris(oxy)] tris(ethane)	Triethoxymethane; Triethyl ester orthoformic acid; Triethyl orthoformate
	6881-94-3	47-060 /S1	2-(2-Propoxyethoxy)ethanol	Diethylene glycol monopropyl ether
$C_7H_{16}S$	1639-09-4	52-017 /B+S1	1-Heptanethiol	1-Heptyl mercaptan
	76858-84-9	51-019	2-(Methylthio)hexane	3-Methyl-2-thiaheptane; Methyl 1-methylpentyl sulfide
$C_7H_{17}NSi$	18387-12-7	71-043	1-[2-(Trimethylsilyl)ethyl]aziridine	*N*-[(*β*-Trimethylsilyl)ethyl] ethylenimine
$C_7H_{18}BrNO$	13186-62-4	75-004 /S2	*N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-propanaminium bromide	
$C_7H_{20}Si_2$	2117-28-4	71-019	Methylenebis(trimethylsilane)	2,2,4,4-Tetramethyl-2,4-disilapentane; Hexamethyldisilamethane; Bis(trimethylsilyl)methane
C_8BrF_{17}	423-55-2	25-050 /S1	1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane	1-Bromoperfluorooctane
C_8D_8	19361-62-7	14-100 /S1	Ethenyl-d_3-benzene-d_5	Styrene-d_8
$C_8D_{14}O_2$	158612-79-4	45-136 /S1	Butyl-d_9 ester 2-(methyl-d_3)-2-propenoic-3,3-d_2 acid	Perdeuterobutyl methacrylate
C_8F_{16}	26637-68-3	21-028	Decafluorobis(trifluoromethyl)cyclohexane	Perfluorodimethylcyclohexane; Hexadecafluorodimethylcyclohexane (unspec. isomer)
$C_8F_{16}O$	646-85-5	61-044	2,2,3,3,4,5,5-Heptafluorotetrahydro-4-(nonafluorobutyl)furan	Perfluoro-3-butyltetrahydrofuran
C_8F_{18}	307-34-6	21-029	Octadecafluorooctane	Perfluorooctane
$C_8F_{18}O_2$	66804-94-2	61-055 /S1	1-[1-[Difluoro(pentafluoroethoxy) methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoropropane	5-Trifluoromethylperfluoro-3,6-dioxanonane
$C_8H_4Cl_2O_2$	88-95-9	61-045	1,2-Benzenedicarbonyl dichloride	Phthaloyl chloride; Phthaloyl dichloride
$C_8H_4N_2$	91-15-6	32-024	1,2-Benzenedicarbonitrile	1,2-Dicyanobenzene; Phthalonitrile
C_8H_6	536-74-3	14-015 /B+S2	Ethynylbenzene	Phenylacetylene
$C_8H_6ClNS_2$	28908-00-1	64-045 /S2	2-[(Chloromethyl)thio]benzothiazole	
C_8H_6O	271-89-6	46-019	Benzofuran	Benzo[*b*]furan; Cumaron
$C_8H_6O_3$	611-73-4	47-061 /S1	*α*-Oxobenzeneacetic acid	Benzoyl formic acid
$C_8H_6O_3Cl_2$	1918-00-9	61-060 /S2	3,6-Dichloro-2-methoxybenzoic acid	3,6-Dichloro-*o*-anisic acid; MDBA; Dicamba
C_8H_6S	95-15-8	53-012	Benzo[*b*]thiophene	
C_8H_7N	140-29-4	32-028 /S1	Benzeneacetonitrile	Phenylacetonitrile; Benzylcyanide
$C_8H_7N_5O_8$	6052-13-7	62-074	*N*-Ethyl-*N*,2,4,6-tetranitrobenzeneamine	Trinitrophenylethylnitroamine; Ethyltetryl

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	43072-20-4	62-075	3-Methyl-2,4,6-trinitro-*N*-(nitromethyl) benzenamine	2,4,6-Trinitro-*N*-(methylnitro)-*m*-toluidine; Methyltetryl
C_8H_8	629-20-9	14-016	1,3,5,7-Cyclooctatetraene	
	100-42-5	14-017	Ethenylbenzene	Vinylbenzene; Styrene
C_8H_8O	496-16-2	46-020	2,3-Dihydrobenzofuran	Coumaran
	496-14-0	46-029 /S1	2,5-Dihydrobenzo-3,4-furan	Phthalan; *o*-Xylylene oxide
	98-86-2	43-036 /B+S1	1-Phenylethanone	Methyl phenyl ketone; Acetophenone; Acetyl benzene; Hypnone
$C_8H_8O_2$	103-82-2	44-038 /S1	Benzeneacetic acid	Phenylacetic acid
	93-58-3	45-048 /B+S1+S2	Methyl benzoate	Methyl ester benzoic acid
	118-90-1	44-017	2-Methylbenzoic acid	*o*-Toluic acid; *o*-Toluylic acid
	99-04-7	44-018	3-Methylbenzoic acid	*m*-Toluic acid
	99-94-5	44-019	4-Methylbenzoic acid	*p*-Toluic acid
$C_8H_8O_3$	119-36-8	47-029	Methyl 2-hydroxybenzoate	Methyl salicylate
	85-43-8	44-020	3*a*,4,7,7*a*-Tetrahydro-1,3-isobenzofurandione	4-Cyclohexene-1,2-dicarboxylic acid anhydride; 1,2,3,6-Tetrahydrophthalic anhydride
	2426-02-0	47-080 /S2	4,5,6,7-Tetrahydro-1,3-isobenzofurandione	1-Cyclohexene-1,2-dicarboxylic anhydride
C_8H_8S	4565-32-6	53-016 /S2	2,3-Dihydrobenzo[*b*]thiophene	1-Thiaindan; Benzothiophane
$C_8H_9NO_2$	614-80-2	62-076	*N*-(2-Hydroxyphenyl)acetamide	*o*-Hydroxyacetanilide
	2603-10-3	62-077	Methyl ester phenylcarbamic acid	Methyl phenylcarbamate; Methyl ester carbanilic acid
C_8H_{10}	95-47-6	14-018/B+S1	1,2-Dimethylbenzene	*o*-Xylene
	108-38-3	14-019 /B+S1+S2	1,3-Dimethylbenzene	*m*-Xylene
	106-42-3	14-020 /B+S1+S2	1,4-Dimethylbenzene	*p*-Xylene
	100-41-4	14-021 /B+S1+S2	Ethylbenzene	Phenylethane
$C_8H_{10}N_2$	935-07-9	34-009	Phenylhydrazone acetaldehyde	
$C_8H_{10}O$	60-12-8	42-066 /B+S2	Benzeneethanol	Phenethyl alcohol; 2-Phenylethanol
	576-26-1	42-127 /S2	2,6-Dimethylphenol	2,6-Xylenol; 1-Hydroxy-2,6-dimethylbenzene
	103-73-1	41-032	Ethoxybenzene	Ethyl phenyl ether; Phenetole
	104-93-8	41-033	1-Methoxy-4-methylbenzene	Methyl 4-methylphenyl ether; *p*-Methylanisole; Methyl *p*-tolyl ether; *p*-Cresol methyl ether
	98-85-1	42-128 /S2	α-Methylbenzenemethanol	(±)-1-Phenylethanol; (*R*,*S*)-α-Phenylethanol
$C_8H_{10}O_2$	91-16-7	41-054 /S2	1,2-Dimethoxybenzene	2-Methoxyanisole; Pyrocatechol dimethyl ether
	122-99-6	47-030	2-Phenoxyethanol	Ethylene glycol monophenyl ether
$C_8H_{10}O_4$	615-99-6	45-049	Di-2-propenyl ethanedioate	Di-2-propenyl ester ethanedioic acid; Diallyl oxalate
$C_8H_{11}Cl_3OS$	76619-94-8	64-039 /S1	*O*-Pentyl ester 2,3,3-trichloro-2-propenethioic acid	*O*-Pentyl ester trichlorothioacrylic acid; *n*-Amyl trichlorothioacrylate
$C_8H_{11}F_6N_3O_4S_2$	174899-82-2	75-005 /S2	1-Ethyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Emim][Tf2N]; [EMim][$CF_3(SO_2)_2$]
$C_8H_{11}N$	64-04-0	31-032	Benzeneethanamine	2-Phenylethylamine; Phenethylamine

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	3211-87-8	32-025 /B+S1	*endo*-Bicyclo[2.2.1]heptane-2-carbonitrile	*endo*-2-Cyanobicyclo[2.2.1] heptane; *endo*-2-Norbornanecarbonitrile
	3211-90-3	32-026 /B+S1	*exo*-Bicyclo[2.2.1]heptane-2-carbonitrile	*exo*-2-Cyanobicyclo[2.2.1] heptane; *exo*-2-Norbornanecarbonitrile
	121-69-7	31-033 /B+S1	*N*,*N*-Dimethylbenzenamine	*N*,*N*-Dimethylaniline
	95-68-1	31-048 /S1	2,4-Dimethylbenzenamine	2,4-Dimethylaniline; 2,4-Xylidine
	95-78-3	31-049 S1	2,5-Dimethylbenzenamine	2,5-Dimethylaniline; 2,5-Xylidine
	87-62-7	31-034 /B+S1	2,6-Dimethylbenzenamine	2,6-Dimethylaniline; 2,6-Xylidine
	103-69-5	31-050 /S1	*N*-Ethylbenzenamine	*N*-Ethylaniline; Ethylphenylamine
	578-54-1	31-051 /S1	2-Ethylbenzenamine	2-Ethylphenylamine; 2-Ethylaniline
	618-36-0	31-052 /S1	α-Methylbenzenemethanamine	α-Methylbenzylamine
	1462-84-6	33-031	2,3,6-Trimethylpyridine	2,3,6-Collidine
	108-75-8	33-032	2,4,6-Trimethylpyridine	2,4,6-Collidine
$C_8H_{11}NO$	156-43-4	62-161 /S1	4-Ethoxybenzenamine	*p*-Phenetidine
C_8H_{12}	931-64-6	14-022	Bicyclo[2.2.2]oct-2-ene	
	111-78-4	14-023	1,5-Cyclooctadiene (unspecified stereoisomer)	
$C_8H_{12}N_2$	929-57-7	34-010	1,6-Diisocyanohexane	1,6-Hexamethylene isocyanide; 1,6-Hexamethylene diisocyanide
$C_8H_{12}N_2O_2$	822-06-0	62-078	1,6-Diisocyanatohexane	Hexamethylene diisocyanate; Hexamethylene ester isocyanic acid
$C_8H_{12}O$	7040-43-9	46-030 /S1	2-(1,1-Dimethylethyl)furan	2-*tert*-Butylfuran
C_8H_{14}	280-33-1	12-020	Bicyclo[2.2.2]octane	
	28282-35-1	12-021	*cis*-Bicyclo[4.2.0]octane	
	931-88-4	14-024	Cyclooctene (unspecified stereoisomer)	
	695-12-5	12-125 /S1	Ethenylcyclohexane	Vinylcyclohexane
	1003-64-1	12-022	Ethylidenecyclohexane	
	765-90-2	12-023	*endo*-2-Methylbicyclo[2.2.1]heptane	*endo*-2-Methylnorbornane
	872-78-6	12-024	*exo*-2-Methylbicyclo[2.2.1]heptane	*exo*-2-Methylnorbornane
	1755-05-1	12-025	*cis*-Octahydropentalene	*cis*-Bicyclo[3.3.0]octane
	5597-89-7	12-026	*trans*-Octahydropentalene	*trans*-Bicyclo[3.3.0]octane
	3524-75-2	12-027	(2-Propenyl)cyclopentane	Allylcyclopentane
$C_8H_{14}O$	110-93-0	43-037	6-Methyl-5-hepten-2-one	
	283-27-2	46-021	3-Oxabicyclo[3.2.2]nonane	
$C_8H_{14}O_2$	97-88-1	45-050 /B+S1	Butyl 2-methyl-2-propenoate	Butyl methacrylate
	622-45-7	45-163 /S2	Cyclohexyl acetate	Cyclohexyl ester acetic acid
	6321-45-5	45-051	2-Propenyl pentanoate	Allyl valerate
$C_8H_{14}O_4$	123-25-1	45-052	Diethyl butanedioate	Diethyl ester butanedioic acid; Diethyl succinate
	615-98-5	45-053	Dipropyl ethanedioate	Dipropyl ester ethanedioic acid; Dipropyl oxalate
	123-80-8	45-054	1,2-Ethanediol dipropionate	1,2-Ethanediyl ester propanoic acid; Ethylene glycol dipropionate
$C_8H_{14}O_6$	87-91-2	47-031	Diethyl ester 2,3-dihydroxy-[*R*-(*R**,*R**)]-butanedioic acid	Diethyl *L*(+)-tartarate
$C_8H_{15}BF_4N_2$	174501-65-6	75-006 /S2	1-Butyl-3-methyl-1*H*-imidazolium tetrafluoroborate	[Bmim][BF_4]
$C_8H_{15}BrN_2$	85100-77-2	75-007 /S2	1-Butyl-3-methyl-1*H*-imidazolium bromide	[Bmim][Br]
$C_8H_{15}ClN_2$	79917-90-1	75-008 /S2	1-Butyl-3-methyl-1*H*-imidazolium chloride	[Bmim][Cl]

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_8H_{15}F_6N_2P$	174501-64-5	75-009 /S2	1-Butyl-3-methyl-1*H*-imidazolium hexafluorophosphate	[Bmim] [PF_6]; [C4mim][PF_6]
$C_8H_{15}N$	283-24-9	33-033	3-Azabicyclo[3.2.2]nonane	
$C_8H_{15}O_2Tl$	18993-50-5	74-027 /S1	Thallium(1+) salt octanoic acid	Thallium(I) octanoate
C_8H_{16}	292-64-8	12-028 /B+S2	Cyclooctane	
	590-66-9	12-029	1,1-Dimethylcyclohexane	
	2207-01-4	12-030	*cis*-1,2-Dimethylcyclohexane	
	6876-23-9	12-031	*trans*-1,2-Dimethylcyclohexane	
	638-04-0	12-032	*cis*-1,3-Dimethylcyclohexane	
	2207-03-6	12-033	*trans*-1,3-Dimethylcyclohexane	
	2207-04-7	12-035	*trans*-1,4-Dimethylcyclohexane	
	1678-91-7	12-036	Ethylcyclohexane	
	111-66-0	13-031	1-Octene	1-Octylene; 1-Caprylene
	2040-96-2	12-037	Propylcyclopentane	
	107-39-1	13-032	2,4,4-Trimethyl-1-pentene	
	107-40-4	13-033	2,4,4-Trimethyl-2-pentene	
$C_8H_{16}O$	123-05-7	43-074 /S2	2-Ethylhexanal	Ethylbutylacetaldehyde; α-Ethylcaproaldehyde
	124-13-0	43-038	Octanal	Octyl aldehyde; Caprilic aldehyde
	111-13-7	43-039	2-Octanone	Hexyl methyl ketone
$C_8H_{16}O_2$	109-21-7	45-055	Butyl butanoate	Butyl butyrate
	123-66-0	45-056	Ethyl hexanoate	Ethyl caproate
	83829-68-9	44-039 /S1	(±)-2-Ethylhexanoic acid	
	142-92-7	45-057 /B+S1	Hexyl acetate	Hexyl ethanoate
	106-73-0	45-058	Methyl heptanoate	Methyl enanthoate
	105-68-0	45-059	3-Methylbutyl propanoate	Isoamyl propionate; Isopentyl propionate
	539-90-2	45-060	2-Methylpropyl butanoate	Isobutyl butyrate
	97-85-8	45-061	2-Methylpropyl 2-methylpropanoate	Isobutyl isobutyrate
	124-07-2	44-021	Octanoic acid	Caprylic acid
	624-54-4	45-062	Pentyl propanoate	Amyl propionate
	141-06-0	45-063	Propyl pentanoate	Propyl valerate
$C_8H_{16}O_4$	112-15-2	47-032	2-(2-Ethoxyethoxy)ethanol acetate	2-(2-Ethoxyethoxy)ethyl acetate; Diethylene glycol ethyl ether acetate
	294-93-9	46-022	1,4,7,10-Tetraoxacyclododecane	
$C_8H_{17}Br$	111-83-1	23-037 /B+S1	1-Bromooctane	*n*-Octyl bromide
$C_8H_{17}Cl$	111-85-3	22-063 /S1+S2	1-Chlorooctane	Octyl chloride
$C_8H_{17}NO$	1116-24-1	62-079	*N*,*N*-Dipropylacetamide	
C_8H_{18}	584-94-1	11-025	2,3-Dimethylhexane	
	592-13-2	11-026	2,5-Dimethylhexane	
	563-16-6	11-027	3,3-Dimethylhexane	
	609-26-7	11-028	3-Ethyl-2-methylpentane	
	592-27-8	11-029	2-Methylheptane	
	589-81-1	11-030	3-Methylheptane	
	589-53-7	11-031	4-Methylheptane	Methyldipropylmethane
	111-65-9	11-032 /B+S1+S2	Octane	
	594-82-1	11-033	2,2,3,3-Tetramethylbutane	
	540-84-1	11-034 /B+S1+S2	2,2,4-Trimethylpentane	Isooctane
	560-21-4	11-035	2,3,3-Trimethylpentane	
	565-75-3	11-036	2,3,4-Trimethylpentane	
$C_8H_{18}N_2O$	16649-52-8	62-080	Bis(1,1-dimethylethyl)diazene 1-oxide	Di-*tert*-butyldiazene *N*-oxide
$C_8H_{18}O$	33021-02-2	41-055 /S2	1-(1,1-Dimethylethoxy)-2-methylpropane	Isobutyl *tert*-butyl ether
	104-76-7	42-067 /B+S1	2-Ethyl-1-hexanol	
	106-67-2	42-068	2-Methyl-1-heptanol	
	625-25-2	42-069	2-Methyl-2-heptanol	
	21570-35-4	42-070	2-Methyl-4-heptanol	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	31367-46-1	42-071	3-Methyl-2-heptanol	
	56298-90-9	42-072	4-Methyl-2-heptanol	
	14979-39-6	42-073	4-Methyl-3-heptanol	
	598-01-6	42-074	4-Methyl-4-heptanol	
	7212-53-5	42-075	5-Methyl-1-heptanol	
	54630-50-1	42-076	5-Methyl-2-heptanol	
	4730-22-7	42-077	6-Methyl-2-heptanol	
	18720-66-6	42-078	6-Methyl-3-heptanol	
	111-87-5	42-079 /B+S1+S2	1-Octanol	Octyl alcohol
	589-98-0	42-081	3-Octanol	
	589-62-8	42-082	4-Octanol	
	142-96-1	41-034 /B+S1	1,1′-Oxybis(butane)	Dibutyl ether
$C_8H_{18}O_2$	110-05-4	47-062 /S1	Bis(1,1-dimethylethyl) peroxide	*tert*-Butyl peroxide
	18854-56-3	41-035	1,2-Dipropoxyethane	4,7-Dioxadecane; Ethylene glycol dipropyl ether
	144-19-4	42-129 /S2	2,2,4-Trimethyl-1,3-pentanediol	TMPD (alcohol)
$C_8H_{18}O_3$	112-34-5	47-033 /B+S1	2-(2-Butoxyethoxy)ethanol	Diethylene glycol monobutyl ether
	112-36-7	41-036	1,1′-Oxybis(2-ethoxyethane)	3,6,9-Trioxaundecane; Diethylene glycol diethyl ether
$C_8H_{18}O_4$	112-49-2	41-037 /B+S1+S2	2,5,8,11-Tetraoxadodecane	Triethylene glycol dimethyl ether; Triglyme
$C_8H_{18}O_5$	112-60-7	47-034 /B+S1	2,2′-[Oxybis(2,1-ethanediyloxy)] bis(ethanol)	Tetraethylene glycol
$C_8H_{18}S$	54063-12-6	51-020	2-(Methylthio)heptane	3-Methyl-2-thiaoctane; Methyl 1-methylhexyl sulfide
	544-40-1	51-021	1,1′-Thiobis(butane)	Dibutyl sulfide
$C_8H_{19}Al$	1191-15-7	73-038 /S1	Hydrobis(2-methylpropyl)aluminum	Diisobutylaluminum hydride
$C_8H_{19}N$	110-96-3	31-035	2-Methyl-*N*-(2-methylpropyl)-1-propanamine	Diisobutylamine
	111-86-4	31-053 /S1+S2	1-Octanamine	Octylamine
$C_8H_{19}NO$	96-80-0	62-162 /S1	2-[Bis(1-methylethyl)aminoethanol	Diisopropylethanolamine; 2-Diisopropylaminoethanol
$C_8H_{19}NO_2$	102-79-4	62-163 /S1	2,2′-(Butylimino)bis(ethanol)	Butyldiethanolamine; 2-[Butyl(2-hydroxyethyl) amino]ethanol
	2160-93-2	62-164 /S1	2,2′-[(1,1-Dimethylethyl)imino] bis(ethanol)	*tert*-Butyldiethanolamine; 2-[*tert*-Butyl(2-hydroxyethyl) amino]ethanol
$C_8H_{19}NSi$	15000-97-2	71-067 /S2	1-(Triethylsilyl)aziridine	Triethylsilylethyleneimine
	42525-64-4	71-020	1-[2-(Trimethylsilyl)ethyl]azetidine	*N*-(*β*-Trimethylsilylethyl) trimethylenimine
$C_8H_{20}BrNO$	28508-15-8	75-010 /S2	*N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-butanaminium bromide	
$C_8H_{20}Ge$	597-63-7	73-024	Tetraethylgermane	
$C_8H_{20}N_4$	6531-38-0	33-034	1,4-Piperazinediethanamine	1,4-Bis(2-aminoethyl) piperazine
	24028-46-4	33-035	*N*-[2-(1-Piperazinyl)ethyl]-1,2-ethanediamine	1-[2-[(2-Aminoethyl)amino] ethyl]piperazine
$C_8H_{20}OZn$	58482-38-5	73-039 /S1	Diethyl[1,1′-oxybis(ethane)]zinc	
$C_8H_{20}O_4Si$	78-10-4	71-021	Tetraethyl ester silicic acid	Tetraethyl orthosilicate; Tetraethoxysilane
$C_8H_{20}Pb$	78-00-2	73-025	Tetraethylplumbane	Tetraethyllead; TEL
$C_8H_{20}Si$	631-36-7	71-022 /B+S1	Tetraethylsilane	
$C_8H_{20}Sn$	597-64-8	73-026	Tetraethylstannane	Tetraethyltin
$C_8H_{20}TeZn$	132851-15-1	73-040 /S1	Diethyl[1,1′-tellurobis(ethane)]zinc	Complex dithylzinc with diethyltellurium
$C_8H_{23}N_5$	112-57-2	31-036	*N*-(2-Aminoethyl)-*N*′-[2-[(2-aminoethyl) amino]ethyl]-1,2-ethanediamine	Tetraethylenepentamine

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_8H_{24}O_2Si_3$	107-51-7	71-063 /S1	Octamethyltrisiloxane	
$C_8H_{24}O_4Si_4$	556-67-2	71-023 /B+S2	Octamethylcyclotetrasiloxane	
$C_8H_{28}N_4Si_4$	1020-84-4	71-024	2,2,4,4,6,6,8,8-Octamethylcyclotetrasilazane	Dimethylaminosilane tetramer
$C_9H_4O_5$	552-30-7	47-035	1,3-Dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid	1,2,4-Benzenetricarboxylic 1:2 anhydride; Trimellitic anhydride
$C_9H_6N_2O_2$	584-84-9	62-081	2,4-Diisocyanato-1-methylbenzene	4-Methyl-*m*-phenyl diisocyanate; 4-Methyl-1,3-phenylene ester isocyanic acid; 2,4-Diisocyanate tolylene
C_9H_7ClO	18365-42-9	61-046	2-Chloro-3-phenyl-2-propenal	α-Chlorocinnamaldehyde
C_9H_7N	119-65-3	33-036	Isoquinoline	Benzo[*c*]pyridine
	91-22-5	33-037	Quinoline	Benzo[*b*]pyridine
C_9H_8	95-13-6	14-025	1*H*-Indene	
$C_9H_8N_2$	7164-98-9	33-053 /S1	1-Phenyl-1*H*-imidazole	
	1126-00-7	33-054 /S1	1-Phenyl-1*H*-pyrazole	
C_9H_8O	104-55-2	43-040	3-Phenyl-2-propenal	Cinnamaldehyde
C_9H_{10}	496-11-7	14-026	2,3-Dihydroindene	Indan
	98-83-9	14-027 /B+S1	(1-Methylethenyl)benzene	Isopropenylbenzene; α-Methylstyrene
$C_9H_{10}N_2$	1075-76-9	34-015 /S2	3-(Phenylamino)propanenitrile	*N*-(2-Cyanoethyl)aniline; 3-Anilinopropionitrile
$C_9H_{10}O$	493-05-0	46-023	3,4-Dihydro-1*H*-2-benzopyran	Isochroman
	493-08-3	46-024	3,4-Dihydro-2*H*-1-benzopyran	Chroman
	93-53-8	43-075 /S2	α-Methylbenzeneacetaldehyde	2-Phenylpropionaldehyde; Hydratropaldehyde
	93-55-0	43-041	1-Phenyl-1-propanone	Ethyl phenyl ketone; Propiophenone
$C_9H_{10}O_2$	93-89-0	45-064 /B+S1+S2	Ethyl benzoate	Ethyl ester benzoic acid
	99-36-5	45-165 /S2	Methyl ester 3-methylbenzoic acid	Methyl *m*-toluate
	99-75-2	45-166 /S2	Methyl ester 4-methylbenzoic acid	Methyl-*p*-toluate
	89-71-4	45-164 /S2	Methyl-2-methylbenzoate	Methyl *o*-toluate
	122-60-1	47-036 /B+S1	(Phenoxymethyl)oxirane	Phenyl glycidyl ether
	140-11-4	45-065	Phenylmethyl acetate	Phenylmethyl ester acetic acid; Benzyl acetate
$C_9H_{10}O_3$	5333-84-6	44-022	3*a*,4,7,7*a*-Tetrahydro-4-methyl-1,3-isobenzofurandione	3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride; 3-Methyl-1,2,3,6-tetrahydrophthalic anhydride
	3425-89-6	47-081 /S2	3a,4,7,7a-Tetrahydro-5-methyl-1,3-isobenzofurandione	4-Methyl-1,2,3,6-tetrahydrophtalic anhydride
$C_9H_{11}N$	635-46-1	33-038	1,2,3,4-Tetrahydroquinoline	
	10500-57-9	33-039	5,6,7,8-Tetrahydroquinoline	2,3-Cyclohexenopyridine
$C_9H_{11}NO$	100-10-7	62-165 /S1	4-(Dimethylamino)benzaldehyde	
$C_9H_{11}NO_2$	101-99-5	62-082	Ethyl ester phenylcarbamic acid	Ethyl phenylcarbamate; Ethyl ester carbanilic acid
C_9H_{12}	3048-64-4	14-101 /S1	5-Ethenylbicyclo[2.2.1]hept-2-ene	5-Vinylnorbornene
	28304-66-7	14-102 /S1	(*Z*)-5-Ethylidenebicyclo[2.2.1]hept-2-ene	*cis*-5-Ethylidene-2-norbornene
	16219-75-3	14-126 /S2	5-Ethylidenebicyclo[2.2.1]hept-2-ene	5-Ethylidene-2-norbornene
	98-82-8	14-028 /B+S1+S2	(1-Methylethyl)benzene	Isopropylbenzene; Cumene
	103-65-1	14-029 /B+S1+S2	Propylbenzene	
	526-73-8	14-030	1,2,3-Trimethylbenzene	Hemimellitene
	95-63-6	14-031	1,2,4-Trimethylbenzene	Pseudocumene
	108-67-8	14-032 /B+S1	1,3,5-Trimethylbenzene	Mesitylene

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_9H_{12}O$	122-97-4	42-083 /B+S2	Benzenepropanol	3-Phenyl-1-propanol; Phenylethyl carbinol; Hydrocinnamyl alcohol
	622-60-6	41-038	1-Ethoxy-4-methylbenzene	Ethyl-4-methylphenyl ether; *p*-Methylphenetole; Ethyl *p*-tolyl ether
	6738-23-4	41-039	1-Methoxy-2,4-dimethylbenzene	Methyl 2,4-dimethylphenyl ether; 2,4-Dimethylanisole
	622-85-5	41-040	Propoxybenzene	Phenyl propyl ether
$C_9H_{13}F_6N_3O_4S_2$	174899-90-2	75-011 /S2	2,3-Dimethyl-1-ethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Emmim][Tf2N]
$C_9H_{13}N$	2038-57-5	31-037	Benzenepropanamine	3-Phenylpropylamine
	585-32-0	31-054 /S1	α,α-Dimethylbenzenemethanamine	α,α-Dimethylbenzylamine
	103-83-3	31-055 /S1	*N*,*N*-Dimethylbenzenemethanamine	*N*,*N*-Dimethylbenzylamine
	643-28-7	31-056 /S1	2-(1-Methylethyl)benzenamine	2-Isopropylphenylamine; 2-Isopropylaniline
	609-72-3	31-038	*N*,*N*,2-Trimethylbenzenamine	*N*,*N*-Dimethyl-*o*-toluidine
$C_9H_{14}O$	20030-30-2	43-042	2,5,6-Trimethyl-2-cyclohexen-1-one	
$C_9H_{14}O_6$	102-76-1	45-066	1,2,3-Propanetriol triacetate	1,2,3-Propanetriyl ester acetic acid; Triacetin
$C_9H_{15}F_3N_2O_3S$	174899-66-2	75-012 /S2	1-Butyl-3-methyl-1*H*-imidazolium trifluoromethanesulfonate	[Bmim][triflate]
C_9H_{16}	13757-43-2	12-038	*cis*-Bicyclo[6.1.0]nonane	
	3452-09-3	13-041 /S2	1-Nonyne	Heptylacetylene
	496-10-6	12-039	Octahydro-1*H*-indene	Hexahydroindan; Hydrindan (unspecified stereoisomer)
	4551-51-3	12-040	*cis*-Octahydro-1*H*-indene	*cis*-Hexahydroindan; *cis*-Hydrindan
	3296-50-2	12-041	*trans*-Octahydro-1*H*-indene	*trans*-Hexahydroindan; *trans*-Hydrindan
	2114-42-3	12-042	(2-Propenyl)cyclohexane	Allylcyclohexane
$C_9H_{16}O_2$	6222-35-1	45-167 /S2	Cyclohexyl ester propanoic acid	Cyclohexyl propionate
	3289-28-9	45-067	Ethyl cyclohexanecarboxylate	Ethyl ester cyclohexanecarboxylic acid
$C_9H_{16}O_4$	1117-19-7	45-068	Dipropyl propanedioate	Dipropyl ester propanedioic acid; Dipropyl malonate
$C_9H_{17}BF_4N_2$	402846-78-0	75-013 /S2	1-Butyl-2,3-dimethyl-1*H*-imidazolium tetrafluoroborate	[Bmmim][BF_4]
$C_9H_{17}F_6N_2P$	227617-70-1	75-014 /S2	1-Butyl-2,3-dimethyl-1*H*-imidazolium hexafluorophsophate	[Bmmim][PF_6]
$C_9H_{17}N$	105728-23-2	33-055 /S1	*trans*-(±)-Decahydroquinoline	*trans*-(*R*,*S*)-Decahydroquinoline
C_9H_{18}	2040-95-1	12-043	Butylcyclopentane	
	124-11-8	13-034 /B+S1	1-Nonene	
	1678-92-8	12-044	Propylcyclohexane	
$C_9H_{18}O$	108-83-8	43-043	2,6-Dimethyl-4-heptanone	Diisobutyl ketone
	124-19-6	43-044	Nonanal	Nonyl aldehyde; Pelargonic aldehyde
	502-56-7	43-045	5-Nonanone	Dibutyl ketone
$C_9H_{18}O_2$	591-68-4	45-069	Butyl pentanoate	Butyl valerate
	112-06-1	45-137 /S1	Heptyl acetate	
	111-11-5	45-070 /B+S2	Methyl octanoate	Methyl caprylate
	106-27-4	45-071	3-Methylbutyl butanoate	Isoamyl butyrate; Isopentyl butyrate
	2050-01-3	45-072	3-Methylbutyl 2-methylpropanoate	Isoamyl isobutyrate; Isopentyl isobutyrate
	10588-10-0	45-073	2-Methylpropyl pentanoate	Isobutyl valerate
	112-05-0	44-023	Nonanoic acid	Pelargonic acid
	540-18-1	45-074	Pentyl butanoate	Pentyl butyrate; Amyl butyrate

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_9H_{18}O_4$	20267-21-4	47-063 /S1	2-(2′-Hydroxyethoxy)ethyl ester 2,2-dimethylpropanoic acid	2-(2′-Hydroxyethoxy)ethyl pivalate
$C_9H_{19}Br$	693-58-3	23-038 /B+S2	1-Bromononane	*n*-Nonyl bromide
$C_9H_{19}Cl$	2473-01-0	22-066 /S2	1-Chlorononane	Nonyl chloride
$C_9H_{19}NOS$	759-94-4	64-026	*S*-Ethyl ester dipropylcarbamothionic acid	*S*-Ethyl dipropylthiocarbamate
C_9H_{20}	1067-20-5	11-037	3,3-Diethylpentane	
	111-84-2	11-038 /B+S1+S2	Nonane	
	7154-79-2	11-039	2,2,3,3-Tetramethylpentane	
	1070-87-7	11-040	2,2,4,4-Tetramethylpentane	
$C_9H_{20}N_2O$	1187-03-7	62-083 /B+S2	Tetraethyl urea	Tetraethylcarbamide
$C_9H_{20}O$	143-08-8	42-084 /B+S1+S2	1-Nonanol	Nonyl alcohol
$C_9H_{20}O_2$	115-84-4	42-130 /S2	2-Butyl-2-ethyl-1,3-propanediol	3,3-Bis(hydroxymethyl)heptane
	2568-90-3	41-056 /S2	1,1′-[Methylenebis(oxy)]bis(butane)	Dibutoxymethane; Dibutyl formal
$C_9H_{20}O_4$	1638-16-0	47-064 /S1	1,1′-[(1-Methyl-1,2-ethanediyl)bis(oxy)] bis(2-propanol)	Tri(propylene glycol)
$C_9H_{21}Al$	102-67-0	73-027 /B+S1	Tripropylaluminum	
$C_9H_{21}As$	5852-57-3	73-056 /S2	Tripropylarsine	
$C_9H_{21}ClO_3Si$	5089-70-3	71-025	(3-Chloropropyl)triethoxysilane	
$C_9H_{21}N$	102-69-2	31-067 /S2	*N*,*N*-Dipropyl-1-propanamine	Tripropylamine; Tri-*n*-propylamine
$C_9H_{23}NO_3Si$	919-30-2	71-026	3-(Triethoxysilyl)-1-propanamine	3-(Triethoxysilyl)propylamine; 3-Aminopropyltriethoxysilane
$C_9H_{24}Si_2$	2295-05-8	71-027	1,3-Propanediylbis(trimethylsilane)	2,2,6,6-Tetramethyl-2,6-disilaheptane; Hexamethyldisilylpropane
$C_9H_{24}Si_3$	1627-99-2	71-028	1,1,3,3,5,5-Hexamethyl-1,3,5-trisilacyclohexane	
$C_{10}F_{16}$	54939-04-7	21-030	Hexadecafluoro-1,2,3,4,5,6,7,8-octahydronaphthalene	
$C_{10}F_{18}$	60433-11-6	21-031	*cis*-Octadecafluorodecahydronaphthalene	*cis*-Perfluorodecaline
	60433-12-7	21-032	*trans*-Octadecafluorodecahydronaphthalene	*trans*-Perfluorodecaline
$C_{10}H_2O_6$	89-32-7	44-024	1*H*,3*H*-Benzo[1,2-*c*:4,5-*c*′]difuran-1,3,5,7-tetrone	1,2,4,5-Benzenetetracarboxylic 1,2:4,5 dianhydride; Pyromellitic dianhydride
$C_{10}H_6O_2S$	49833-12-7	63-005	1-Oxide naphtho[1,8-*cd*]-1,2-dithiole	Naphthalene 1,8-disulfide-*S*-oxide
$C_{10}H_7Cl$	90-13-1	22-044 /B+S1	1-Chloronaphthalene	
	91-58-7	22-045	2-Chloronaphthalene	
$C_{10}H_7NO_2$	86-57-7	62-084	1-Nitronaphthalene	α-Nitronaphthalene
$C_{10}H_8$	91-20-3	14-033 /B+S1+S2	Naphthalene	
$C_{10}H_8O$	90-15-3	42-085	1-Naphthol	α-Naphthol
	135-19-3	42-086 /B+S2	2-Naphthol	β-Naphthol
$C_{10}H_9N$	91-63-4	33-058 /S2	2-Methylquinoline	
	611-32-5	33-059 /S2	8-Methylquinoline	
	134-32-7	31-057 /S1	1-Naphthalenamine	1-Aminonaphthalene; α-Naphthylamine
	91-59-8	31-039	2-Naphthalenamine	β-Naphthalenamine; 2-Aminonaphthalene
$C_{10}H_{10}$	1005-51-2	14-034	Tricyclo[3.3.2.0^{2,8}]deca-3,6,9-triene	
$C_{10}H_{10}Fe$	102-54-5	73-028	Ferrocene	Dicyclopentadienyliron
$C_{10}H_{10}N_2$	10199-67-4	33-056 /S1	1-(Phenylmethyl)-1*H*-pyrazole	1-Benzylpyrazole
$C_{10}H_{10}O$	529-34-0	43-066 /S1	3,4-Dihydro-1(2*H*)-naphthalenone	α-Tetralone; 1,2,3,4-Tetrahydro-1-naphthalenone
	101-39-3	43-076 /S2	2-Methyl-3-phenyl-2-propenal	α-Methyl cinnamaldehyde
$C_{10}H_{10}O_2$	1754-62-7	45-168 /S2	(2*E*)-Methyl ester 3-phenyl-2-propenoic acid	*trans*-Methyl cinnamate
	583-04-0	45-075	2-Propenyl benzoate	2-Propenyl ester benzoic acid; Allyl benzoate

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{10}H_{10}O_4$	131-11-3	45-076 /B+S1+S2	Dimethyl 1,2-benzenedicarboxylate	Dimethyl phthalate; Dimethyl ester 1,2-benzenedicarboxylic acid
	120-61-6	45-077	Dimethyl 1,4-benzenedicarboxylate	Dimethyl terephthalate; Dimethyl ester 1,4-benzenedicarboxylic acid
	1459-93-4	45-138 /S1	Dimethyl ester 1,3-benzenedicarboxylic acid	Dimethyl isophthalate
$C_{10}H_{12}$	2039-93-2	14-103 /S1	1-Methylenepropylbenzene	α-Ethylstyrene
	1755-01-7	14-104 /S1	(3aα,4α,7α,7aα)-3a,4,7,7a-Tetrahydro-4,7-methano-1*H*-indene	*endo*-Dicyclopentadiene
	119-64-2	14-035 /B+S1	1,2,3,4-Tetrahydronaphthalene	Tetralin
$C_{10}H_{12}O$	937-30-4	43-046	1-(4-Ethylphenyl)ethanone	4′-Ethylacetophenone
	104-46-1	41-041	1-Methoxy-4-(1-propenyl)benzene	*p*-Propenylanisole; Anethole
$C_{10}H_{12}O_2$	97-53-0	47-037	2-Methoxy-4-(2-propenyl)phenol	4-Allyl-2-methoxyphenol; Eugenol
	2315-68-6	45-078	Propyl benzoate	Propyl ester benzoic acid
$C_{10}H_{13}NO_2$	5532-90-1	62-085	Propyl ester phenylcarbamic acid	Propyl phenylcarbamate; Propyl ester carbanilic acid
$C_{10}H_{14}$	104-51-8	14-036 /B+S2	Butylbenzene	1-Phenylbutane
	98-06-6	14-037 /B+S2	(1,1-Dimethylethyl)benzene	*tert*-Butylbenzene; 2-Methyl-2-phenylpropane
	99-87-6	14-038	1-Methyl-4-(1-methylethyl)benzene	1-Isopropyl-4-methylbenzene; *p*-Cymene
	135-98-8	14-039 /B+S2	(1-Methylpropyl)benzene	*sec*-Butylbenzene; 2-Phenylbutane
	538-93-2	14-127 /S2	(2-Methylpropyl)benzene	Isobutylbenzene
	488-23-3	14-040	1,2,3,4-Tetramethylbenzene	Prehnitene
	527-53-7	14-041	1,2,3,5-Tetramethylbenzene	Isodurene
	95-93-2	14-042 /B+S2	1,2,4,5-Tetramethylbenzene	Durene
$C_{10}H_{14}O$	88-18-6	42-112 /S1	2-(1,1-Dimethylethyl)phenol	2-*tert*-Butylphenol; 1-*tert*-Butyl-2-hydroxybenzene
	22327-39-5	43-067 /S1	(±)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	(±)-*p*-Mentha-6,8-dien-2-one; *dl*-Carvone
	6485-40-1	43-068 /S1	(*R*)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	(*R*)-*p*-Mentha-6,8-dien-2-one; *l*-Carvone
	499-75-2	42-087	2-Methyl-5-(1-methylethyl)phenol	5-Isopropyl-2-methylphenol; Carvacrol
	700-58-3	43-077 /S2	Tricyclo[3.3.1.1^{3,7}]decanone	2-Adamantanone
$C_{10}H_{14}O_2$	98-29-3	42-113 /S1	4-(1,1-Dimethylethyl)-1,2-benzenediol	4-*tert*-Butylcatechol; 4-*tert*-Butylpyrocatechol
$C_{10}H_{14}O_4$	925-16-6	45-079	Di-2-propenyl butanedioate	Di-2-propenyl ester butanedioic acid; Diallyl succinate
$C_{10}H_{14}Si$	3944-08-9	71-064 /S1	1-Methyl-1-phenylsilacyclobutane	
	1125-26-4	71-029	Ethenyldimethylphenylsilane	
$C_{10}H_{15}Br$	768-90-1	23-047 /S2	1-Bromotricyclo[3.3.1.1^{3,7}]decane	1-Bromoadamantane
$C_{10}H_{15}F_6N_3O_4S_2$	174899-83-3	75-015 /S2	1-Butyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide	[Bmim][Tf2N]
	169051-76-7	75-016 /S2	2,3-Dimethyl-1-propyl-1*H*-imidazolium bis(trifluoromethylsulfonyl)imide	[Pmmim][Tf2N]
$C_{10}H_{15}N$	91-66-7	31-040	*N*,*N*-Diethylbenzenamine	*N*,*N*-Diethylaniline
	579-66-8	31-058 /S1	2,6-Diethylbenzenamine	2,6-Diethylphenylamine; 2,6-Diethylaniline
	6310-21-0	31-059 /S1	2-(1,1-Dimethylethyl)benzenamine	2-*tert*-Butylphenylamine; 2-*tert*-Butylaniline
$C_{10}H_{15}NO$	55658-55-4	62-086	(*E*)-(*R*,*S*)-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime	*dl*-Carvoxime

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	60827-56-7	62-087	[*R*-(*E*)]-2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one oxime	*l*-Carvoxime
$C_{10}H_{15}N_5$	448245-52-1	75-017 /S2	1-Butyl-3-methyl-1*H*-imidazolium dicyanamide	[Bmim][dca]
$C_{10}H_{16}$	127-91-3	12-045 /B+S1	6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane	β-Pinene; Nopinene; Terebenthene
	138-86-3	14-043 /B+S1	1-Methyl-4-(1-methylethenyl)cyclohexene	Limonene
	5989-27-5	14-105 /S1+S2	(4*R*)-1-Methyl-4-(1-methylethenyl) cyclohexene	*d*-Limonene
	3387-41-5	12-046	4-Methylene-1-(1-methylethyl)bicyclo[3.1.0] hexane	Sabinene
	6004-38-2	12-047 /B+S2	Octahydro-4,7-methano-1*H*-indene	Hexahydro-4,7-methanoindan; Tricyclo[5.2.1.0^{2,6}]decane; Tetrahydrodicyclopentadiene
	2825-82-3	12-126 /S1+S2	(3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene	*exo*-Tetrahydrodicyclopentadiene
	281-23-2	12-127 /S1	Tricyclo[3.3.1.1^{3,7}]decane	Adamantane
	80-56-8	14-106 /S1	2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	α-Pinene; (*dl*)-Pin-2-ene
	7785-70-8	14-128 /S2	(1*R*,5*R*)-2,6,6-Trimethylbicyclo[3.1.1] hept-2-ene	(+)-α-Pinene; (1*R*,5*R*)(+)α-Pinene
	7785-26-4	14-129 /S2	(1*S*,5*S*)-2,6,6-Trimethylbicyclo[3.1.1] hept-2-ene	(-)-α-Pinene; (1*S*,5*S*)-(-)-α-Pinene
$C_{10}H_{16}BF_4N$	597581-48-1	75-018 /S2	1-Butyl-3-methylpyridinium tetrafluoroborate	[Bmpy][BF_4]
$C_{10}H_{16}O$	76-22-2	43-047	Camphor	1,7,7-Trimethylbicyclo[2.2.1] heptan-2-one
	5392-40-5	43-048	3,7-Dimethyl-2,6-octadienal	Citral
	29171-20-8	42-088	3,7-Dimethyl-6-octen-1-yn-3-ol	Dehydrolynalol
	15932-80-6	43-049	5-Methyl-2-(1-methylethylidene) cyclohexanone	*p*-Menth-4(8)-en-3-one; 1-Isopropylidene-4-methylcyclohexan-2-on; Pulegone
	768-95-6	42-131 /S2	Tricyclo[3.3.1.1^{3,7}]decan-1-ol	1-Adamantanol
	700-57-2	42-132 /S2	Tricyclo[3.3.1.1^{3,7}]decan-2-ol	2-Adamantanol
$C_{10}H_{16}O_2$	10453-89-1	44-044 /S2	2,2-Dimethyl-3-(2-methyl-1-propenyl) cyclopropanecarboxylic acid	Chrysanthemic acid
$C_{10}H_{17}NO_4S$	872672-50-9	75-019 /S2	1-Ethyl-3-methylpyridinium ethyl sulfate	[Empy][$EtSO_4$]
$C_{10}H_{18}$	1636-39-1	12-048 /B+S2	1,1′-Bicyclopentyl	Cyclopentylcyclopentane
	16189-46-1	12-049	*cis*-Decahydroazulene	*cis*-Perhydroazulene; *cis*-Bicyclo[5.3.0]decane
	91-17-8	12-050	Decahydronaphthalene	Decalin (unspec. isomer)
	493-01-6	12-051	*cis*-Decahydronaphthalene	*cis*-Decalin
	493-02-7	12-052	*trans*-Decahydronaphthalene	*trans*-Decalin
		12-053	Octahydromethyl-1*H*-indene	Hexahydromethylindan; Methylhydrindan (unspec. isomer)
	473-55-2	12-054	2,6,6-Trimethylbicyclo[3.1.1]heptane	Pinane
$C_{10}H_{18}F_6N_2O_4S_2$	223437-05-6	75-020 /S2	1-Methyl-1-propylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide	[MPPyN(CF_3SO_2)$_2$]
$C_{10}H_{18}O$	78-70-6	42-089	3,7-Dimethyl-1,6-octadien-3-ol	Linalol
$C_{10}H_{18}O_2$	1551-44-6	45-169 /S2	Cyclohexyl ester butanoic acid	Cyclohexyl butyrate
$C_{10}H_{18}O_3$	1538-75-6	44-045 /S2	2,2-Dimethylpropanoic acid anhydride	Pivalic anhydride
$C_{10}H_{18}O_4$	2050-61-5	45-080	Bis(2-methylpropyl) ethanedioate	Bis(2-methylpropyl) ester ethanedioic acid; Diisobutyl oxalate
	925-15-5	45-081	Dipropyl butanedioate	Dipropyl ester butanedioic acid; Dipropyl succinate

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	105-72-6	45-082	1,2-Ethanediyl dibutanoate	1,2-Ethanediyl ester butanoic acid; 1,2-Ethanediol dibutyrate; Ethylene glycol dibutyrate
$C_{10}H_{18}Si$	17985-13-6	71-065 /S1	Bicyclo[2.2.1]hept-5-en-2-yltrimethylsilane	5-Trimethylsilyl-2-norbornene
$C_{10}H_{19}BF_4N_2$	244193-50-8	75-021 /S2	1-Hexyl-3-methy-1*H*-imidazolium tetrafluoroborate	[Hmim][BF_4]
$C_{10}H_{19}BrN_2$	85100-78-3	75-022 /S2	1-Hexyl-3-methyl-1*H*-imidazolium bromide	[Hmim][Br]
$C_{10}H_{19}F_6N_2P$	304680-35-1	75-023 /S2	1-Hexyl-3-methyl-1*H*-imidazolium hexafluorophosphate	[Hmim][PF_6]; [C6mim][PF_6][PF_6]
$C_{10}H_{20}$	1678-93-9	12-055	Butylcyclohexane	
	293-96-9	12-138 /S2	Cyclodecane	
	872-05-9	13-035 /B+S1	1-Decene	1-Decylene; α-Decylene
	1331-43-7	12-056	Diethylcyclohexane (unspecifiedisomer)	
	1679-00-1	12-057	1,4-Diethylcyclohexane	
	3178-22-1	12-058	(1,1-Dimethylethyl) cyclohexane	*Tert*-Butylcyclohexane
$C_{10}H_{20}O$	112-31-2	43-050	Decanal	Decyl aldehyde; Capric aldehyde
	89-78-1	42-114 /S1	(1α,2β,5α)-5-Methyl-2-(1-methylethyl) cyclohexanol	(±)-Menthol; *p*-Menthan-3-ol; (±)-2-Isopropyl-5-methylcyclohexanol
$C_{10}H_{20}O_2$	334-48-5	44-025	Decanoic acid	Capric acid
	2639-63-6	45-083	Hexyl butanoate	Hexyl butyrate
	1731-84-6	45-170 /S2	Methyl nonanoate	Methyl pelargonate
	2050-09-1	45-084	3-Methylbutyl pentanoate	Isoamyl valerate; Isopentyl valerate
	112-14-1	45-085 /B+S1+S2	Octyl acetate	
$C_{10}H_{20}O_4$	124-17-4	47-038	2-(2-Butoxyethoxy)ethanol acetate	2-(2-Butoxyethoxy)ethyl acetate; Diethylene glycol butyl ether acetate
$C_{10}H_{20}O_5$	33100-27-5	46-025	1,4,7,10,13-Pentaoxacyclopentadecane	
$C_{10}H_{21}Br$	112-29-8	23-048 /S2	1-Bromodecane	Decyl bromide
$C_{10}H_{21}Cl$	1002-69-3	22-067 /S2	1-Chlorodecane	Decyl chloride
$C_{10}H_{21}NO$	1563-90-2	62-088	*N*,*N*-Dibutylacetamide	
$C_{10}H_{22}$	124-18-5	11-041 /B+S1+S2	Decane	Decyl hydride
	1072-16-8	11-042	2,7-Dimethyloctane	
	871-83-0	11-043	2-Methylnonane	Isodecane
	5911-04-6	11-044	3-Methylnonane	
	17301-94-9	11-045	4-Methylnonane	
	15869-85-9	11-046	5-Methylnonane	
$C_{10}H_{22}N_4$	19479-83-5	33-040	1,1′-(1,2-Ethanediyl)bis(piperazine)	Dipiperazinylethane
$C_{10}H_{22}O$	112-30-1	42-090 /B+S1+S2	1-Decanol	Decyl alcohol
	5205-34-5	42-091	5-Decanol	
	106-21-8	42-092	3,7-Dimethyl-1-octanol	
	33933-78-7	42-133 /S2	5-Methyl-5-nonanol	2-Butyl-2-hexanol
	2198-72-3	42-093	4-Propyl-4-heptanol	
$C_{10}H_{22}O_2$	112-47-0	42-115 /S1	1,10-Decanediol	
	112-48-1	41-042	1,1′-[1,2-Ethanediylbis(oxy)]bis(butane)	1,2-Dibutoxyethane; Ethylene glycol dibutyl ether
	871-22-7	41-043	1,1′-[Ethylidenebis(oxy)]bis(butane)	1,1-Dibutoxyethane; Acetaldehyde dibutylacetal; 6-Methyl-5,7-dioxaundecane
$C_{10}H_{22}O_3$	112-59-4	47-082 /S2	2-[2-(Hexyloxy)ethoxy]ethanol	Diethylene glycol hexyl ether
$C_{10}H_{22}O_5$	143-24-8	41-044 /B+S1	2,5,8,11,14-Pentaoxapentadecane	Bis(methoxyethoxyethyl) ether; Tetraethylene glycol dimethyl ether
$C_{10}H_{22}O_6$	4792-15-8	47-039	3,6,9,12-Tetraoxatetradecane-1,14-diol	Pentaethylene glycol
$C_{10}H_{22}S$	143-10-2	52-018 /B+S1	1-Decanethiol	1-Decyl mercaptan

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	3698-94-0	51-029 /S1	1-Ethylthiooctane	Ethyl *n*-octyl sulfide
	872-10-6	51-022	1,1′-Thiobis(pentane)	6-Thiaundecane; Dipentyl sulfide
$C_{10}H_{22}Te$	71475-88-2	73-041 /S1	1,1′-Tellurobis(pentane)	
$C_{10}H_{23}N$	2016-57-1	31-061 /S1+S2	1-Decanamine	*n*-Decylamine
	7378-99-	31-060 /S1	*N*,*N*-Dimethyloctanamine	Dimethyloctylamine
$C_{10}H_{24}BrNO$	219787-58-3	75-024 /S2	*N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-hexanaminium bromide	
$C_{10}H_{24}N_4$	996-70-3	31-062 /S1	Octamethylethenetetramine	Tetrakis(dimethylamino) ethylene
$C_{10}H_{25}N_5$	31295-54-2	33-041	*N*-(2-Aminoethyl)-1,4-piperazine-diethanamine	1-(2-Aminoethyl)-4-[2-[(2-aminoethyl) amino]ethyl]piperazine
$C_{10}H_{25}O_5U$		73-042 /S1	Pentaethoxyuranium	Uranium pentaethylate
$C_{10}H_{26}O_3Si_3$	110505-51-6	71-030	2,2,4,4-Tetraethyl-6,6-dimethylcyclo-trisiloxane	
$C_{10}H_{30}O_5Si_5$	541-02-6	71-068 /S2	Decamethylcyclopentasiloxane	Dimethylsiloxane pentamer
$C_{11}H_{10}$	90-12-0	14-044	1-Methylnaphthalene	α-Methylnaphthalene
	91-57-6	14-045	2-Methylnaphthalene	β-Methylnaphthalene
$C_{11}H_{12}O_2$	103-36-6	45-086	Ethyl 3-phenyl-2-propenoate	Ethyl ester 3-phenyl-2-propenoic acid; Ethyl cinnamate (unspecified stereoisomer)
	40317-63-3	45-139 /S1	Methyl ester pentacyclo[4.3.0.0^{2,5}.0^{3,8}.0^{4,7}]nonane-4-carboxylic acid	4-Carbomethoxyhomocubane
	2495-37-6	45-087	Phenylmethyl 2-methyl-2-propenoate	Phenylmethyl ester 2-methyl-2-propenoic acid; Benzyl methacrylate
$C_{11}H_{14}$	4912-92-9	14-046	1,1-Dimethylindan	
	1685-82-1	14-047	4,6-Dimethylindan	
	6682-1-9	14-048	4,7-Dimethylindan	
	17498-71-4	14-107 /S1	(2-Methyl-1-methylenepropyl)benzene	α-Isopropylstyrene
	4421-32-3	12-128 /S1	Octahydro-1,2,4-ethanylylidene-1*H*-cyclobuta[*c*,*d*]pentalene	Pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane
$C_{11}H_{14}F_6N_2O_4S_2$	187863-42-	75-025 /S2	1-Butyl-pyridinium bis(trifluoromethylsulfonyl)imid	1-Butyl-pyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide; [BPy][BTI]
$C_{11}H_{14}O_2$	136-60-7	45-140 /S1	Butyl benzoate	
	2021-28-5	45-088	Ethyl benzenepropanoate	Ethyl ester benzenepropanoic acid; Ethyl 3-phenylpropanoate; Ethyl hydrocinnamate
$C_{11}H_{14}O_3$	614-45-9	47-065 /S1	1,1-Dimethylethyl ester benzenecarboperoxoic acid	*Tert*-Butyl peroxybenzoate;*tert*-Butyl perbenzoate
$C_{11}H_{15}F_6N_3O_4S_2$	900797-77-5	75-026 /S2	*N*-Ethyl-4-4(*N*′,*N*′-dimethylammonium) pyridinium bis(trifluoromethylsulfonyl)imid	[EAPy][BTI]
$C_{11}H_{16}$	700-12-9	14-049	Pentamethylbenzene	
$C_{11}H_{16}O$	88-60-8	42-116 /S1	2-(1,1-Dimethylethyl)-5-methylphenol	2-*tert*-Butyl-5-methylphenol
$C_{11}H_{16}Si$	18001-46-2	71031	Ethenyldimethyl(phenylmethyl)silane	Benzyldimethylvinylsilane
$C_{11}H_{18}O$	702-98-7	42-134 /S2	2-Methyltricyclo[3.3.1.1^{3,7}]decan-2-ol	2-Methyl-2-adamantanol
$C_{11}H_{19}F_3N_2O_3S$	460345-16-8	75-027 /S2	1-Hexyl-3-methylimidazolium trifluoromethanesulfonate	1-Hexyl-3-methylimidazolium trifluoromethanesulfonic acid; [Hmim][OTf]
$C_{11}H_{19}NO_2$	62391-95-1	62166 /S1	Ethyl ester 2-cyano-3-methyl-2-(1-methylethyl) butanoic acid	Ethyl ester 2-cyano-2-isopropyl-3-methylbutyric acid
$C_{11}H_{20}$	2958-75-0	12-059	Decahydro-1-methylnaphthalene	α-Methyldecalin
	2958-76-1	12-060	Decahydro-2-methylnaphthalene	β-Methyldecalin
	95098-51-4	12-061	Ethyloctahydro-1*H*-indene	Ethylhexahydroindan; Ethylhydrindan (unspecified isomer)

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{11}H_{20}O_2$	1551-43-5	45-171 /S2	Cyclohexyl ester pentanoic acid	Cyclohexyl valerate
	1725-03-7	47-040	Oxacyclododecan-2-one	Undecanolide; Undecanolactone
$C_{11}H_{22}$	821-95-4	13-036	1-Undecene	α-Undecene
$C_{11}H_{22}O_2$	110-42-9	45-089 /B+S2	Methyl decanoate	Methyl caprate
	143-13-5	45-141 /S1	Nonyl acetate	
	112-37-8	44-026	Undecanoic acid	Undecylic acid
$C_{11}H_{24}$	6975-98-0	11-047	2-Methyldecane	
	1120-21-4	11-048 /B+S2	Undecane	Hendecane
$C_{11}H_{24}O$	7289-52-3	41-045	1-Methoxydecane	Decyl methyl ether
	112-42-5	42-094 /B+S2	1-Undecanol	Undecyl alcohol; Decyl carbinol; 1-Hendecanol
$C_{12}F_{10}$	434-90-2	21-033	2,2′,3,3′,4,4′,5,5′,6,6′-Decafluoro-1,1′-biphenyl	Decafluorobiphenyl; Perfluorobiphenyl
$C_{12}F_{26}$	307-59-5	21-052 /S1	Hexacosafluorododecane	Perfluorododecane
$C_{12}H_4Cl_4O_2$	30746-58-8	61-061 /S2	1,2,3,4-Tetrachlorodibenzo[*b*,*e*][1,4]dioxin	1,2,3,4-TCDD
$C_{12}H_8$	208-96-8	14-050	Acenaphthylene	
$C_{12}H_8Cl_2O_2S$	80-07-9	64-027	1,1′-Sulfonylbis(4-chlorobenzene)	Bis(*p*-chlorophenyl)sulfone; 4,4′-Dichlorodiphenyl sulfone
$C_{12}H_8N_2O_5$	101-63-3	62-089	1,1′-Oxybis(4-nitrobenzene)	Bis(*p*-nitrophenyl) ether; 4,4′-Dinitrodiphenyl ether
$C_{12}H_8O$	132-64-9	46-026 /B+S1	Dibenzofuran	Diphenylene oxide
$C_{12}H_8OS$	262-20-4	63-007 /S1	Phenoxathiin	
$C_{12}H_8OS_2$	49833-13-8	63-006	Dibenzo[*c*,*e*][1,2]dithiin-5-oxide	Diphenylene 2,2′-disulfide-*S*-oxide
$C_{12}H_8O_2$	262-12-4	46-032 /S2	Dibenzo[*b*,*e*][1,4]dioxin	Dibenzo-*p*-dioxin; Oxanthrene
$C_{12}H_8S$	132-65-0	53-013 /B+S1	Dibenzothiophene	
$C_{12}H_8S_2$	92-85-3	53-014 /S1	Thianthrene	
$C_{12}H_9Cl$	2051-60-7	22-046	2-Chloro-1,1′-biphenyl	*o*-Chlorobiphenyl; *o*-Chlorodiphenyl
	2051-62-9	22-047	4-Chloro-1,1′-biphenyl	*p*-Chlorobiphenyl; *p*-Chlorodiphenyl
$C_{12}H_9Cl_3Si$	18030-62-1	71-032	[1,1′ -Biphenyl]-2-yltrichlorosilane	*o*-(Trichlorosilyl)biphenyl; *o*-Trichlorosilanediphenyl
	18030-61-0	71-033	[1,1′-Biphenyl]-4-yltrichlorosilane	*p*-(Trichlorosilyl)biphenyl; *p*-Trichlorosilanediphenyl
$C_{12}H_9NO$	91-02-1	62-182 /S2	Phenyl-2-pyridinylmethanone	2-Benzoylpyridine; Phenyl-2-pyridyl ketone
$C_{12}H_{10}$	83-32-9	14-051	Acenaphthene	1,8-Dihydroacenaphthalene; Ethylenenaphthalene
	92-52-4	14-052 /B+S1	1,1′-Biphenyl	Diphenyl
$C_{12}H_{10}F_{15}N_3O_4S_2$	872672-61-2	75-028 /S2	1-Methyl-3-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[perfluoro-hmim][Tf2N]
$C_{12}H_{10}N_2$	103-33-3	34-011 /B+S1	Diphenyldiazene	Azobenzene; Diphenyldiimide (unspecified stereoisomer)
	17082-12-1	34-012 /B+S1	(*E*)-Diphenyldiazene	*trans*-Azobenzene; *trans*-Diphenyldiimide
$C_{12}H_{10}N_2O$	495-48-7	62-167 /S1	1-Oxide diphenyldiazene	*N*,*N*-Diphenyldiazene *N*-oxide; Azoxybenzene
$C_{12}H_{10}O$	101-84-8	41-046	1,1′-Oxybis(benzene)	Diphenyl ether; Diphenyl oxide
$C_{12}H_{10}S$	139-66-2	51-023 /B+S1	1,1′-Thiobis(benzene)	Diphenyl sulfide; Phenyl sulfide
$C_{12}H_{10}Te$	1202-36-4	73-043 /S1	Diphenyltelluride	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{12}H_{11}N$	90-41-5	31-041	(1,1′-Biphenyl)-2-amine	2-Aminobiphenyl
	122-39-4	31-042 /B+S1	*N*-Phenylbenzenamine	Diphenylamine
$C_{12}H_{12}$	569-41-5	14-053	1,8-Dimethylnaphthalene	
	581-400-8	14-054	2,3-Dimethylnaphthalene	
	581-42-0	14-055	2,6-Dimethylnaphthalene	
	582-16-1	14-056 /B+S1	2,7-Dimethylnaphthalene	
$C_{12}H_{12}Ge$	1675-58-7	73-029	Diphenylgermane	
$C_{12}H_{12}N_2O$	101-80-4	62-090	4,4′-Oxybis(benzenamine)	4,4′-Oxydianiline; 4,4′-Diaminodiphenyl ether
$C_{12}H_{12}N_2O_2S$	80-08-0	64-028	4,4′-Sulfonylbis(benzenamine)	4,4′-Sulfonyldianiline; 4-Aminophenyl sulfone; Dapsone
$C_{12}H_{12}S$	16587-33-0	53-017 /S2	1,2,3,4-Tetrahydrodibenzothiophene	
$C_{12}H_{13}NO_2S$	5234-68-4	64-046 /S2	5,6-Dihydro-2-methyl-*N*-phenyl-1,4-oxathiin-3-carboxamide	Carboxine
$C_{12}H_{14}Fe$	1273-89-8	73-057 /S2	Ethylferrocene	Cyclopentadienyl (ethylcyclopentadienyl) iron
$C_{12}H_{14}N_4O$	2676-59-7	62-168 /S1	4,4′-Oxybis(1,2-benzenediamine)	3,3′,4,4′-Tetraaminodiphenyl oxide; 3,3′,4,4′-Tetraaminodiphenyl ether
$C_{12}H_{14}O_4$	84-66-2	45-090 /B+S1+S2	Diethyl 1,2-benzenedicarboxylate	Diethyl phthalate; Diethyl ester 1,2-benzenedicarboxylic acid
	636-09-9	45-091	Diethyl 1,4-benzenedicarboxylate	Diethyl terephthalate; Diethyl ester 1,4-benzenedicarboxylic acid
	131-70-4	45-142 /S1	Monobutyl ester 1,2-benzenedicarboxylic acid	Monobutyl phthalate
$C_{12}H_{15}F_9N_2O_6S_2$	731774-32-6	75-029 /S2	1-Butyl-3-methyl-1*H*-imidazolium tris[(trifluoromethyl)sulfonyl]methane	[Bmim][methide]
$C_{12}H_{16}$	827-52-1	14-057	Cyclohexylbenzene	Phenylcyclohexane
	5676-29-9	14-108 /S1	(2,2-Dimethyl-1-methylenepropyl)benzene	*α-tert*-Butylstyrene
$C_{12}H_{16}F_6N_2O_4S_2$	344790-86-9	75-030 /S2	1-Butyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide	[Bmpy][Tf2N]
$C_{12}H_{18}$	99-62-7	14-109 /S1	1,3-Bis(1-methylethyl)benzene	1,3-Diisopropylbenzene; *m*-Diisopropylbenzene
	100-18-5	14-110 /S1+S2	1,4-Bis(1-methylethyl)benzene	1,4-Diisopropylbenzene; *p*-Diisopropylbenzene
	706-31-0	14-058	(*E*,*E*,*Z*)-1,5,9-Cyclododecatriene	*trans*,*trans*,*cis*-1,5,9-Cyclododecatriene
		12-062	Decahydrodimethanonaphthalene	Dimethanodecalin (unspecified isomer)
	87-85-4	14-059	Hexamethylbenzene	Mellitene
	1077-16-3	14-060 /B+S2	Hexylbenzene	1-Phenylhexane
	102-25-0	14-111 /S1	1,3,5-Triethylbenzene	
$C_{12}H_{18}O$	2078-54-8	42-117 /S1	2,6-Bis(1-methylethyl)phenol	2,6-Diisopropylphenol
	1879-09-0	42-118 /S1	2-(1,1-Dimethylethyl)-4,6-dimethylphenol	2-*tert*-Butyl-4,6-dimethylphenol
$C_{12}H_{19}F_6N_3O_4S_2$	382150-50-7	75-031 /S2	1-Hexyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide	[Hmim][Tf2N]; [Hmim][BTl]
$C_{12}H_{19}N$	24544-04-5	31-063 /S1	2,6-Bis(1-methylethyl)benzenamine	2,6-Diisopropylphenylamine; 2,6-Diisopropylaniline
$C_{12}H_{19}NO_5S$	872672-51-0	75-032 /S2	3-(Ethoxycarbonyl)-1-ethylpyridinium ethyl sulfate	[Et2Nic]
$C_{12}H_{20}$	702-79-4	12-063 /B+S1+S2	1,3-Dimethyltricyclo [3.3.1.1^{3,7}] decane	1,3-Dimethyladamantane
	2146-36-3	12-129 /S1	Dodecahydroacenaphthylene	Perhydroacenaphthylene; Tricyclo [7.2.1.0^{5,12}] dodecane (mixture of stereoisomers)
	770-69-4	12-139 /S2	1-Ethyltricyclo [3.3.1.1^{3,7}] decane	1-Ethyladamantane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	28014-61-1	12-130 /S1	(3aα,4β,7β,7aα)-Octahydrodimethyl-4,7-methano-1*H*-indene	*exo*-Tetrahydrodi (methylcyclopentadiene)
	281-84-5	12-064	Tricyclo [6.2.1.1^{3,6}] dodecane	
$C_{12}H_{20}BrN$	67021-56-1	75-033 /S2	1-Hexyl-3-methylpyridinium bromide	[Hmpy][Br]
$C_{12}H_{20}N_2O_2$	63254-50-2	62-183 /S2	(1*R*,2*S*,5*R*)-5-Methyl-2-(1-methylethyl)cyclohexyl ester diazoacetic acid	1-Methyl diazoacetate
$C_{12}H_{20}OC_{12}H_{20}O$	4789-40-6	46-031 /S1	2,5-Bis(1,1-dimethylethyl)furan	2,5-Di-*tert*-butylfuran
$C_{12}H_{20}O_2$	28746-99-8	47-083 /S2	1′-Hydroxy[1,1′-bicyclohexyl]-2-one	2-(1-Hydroxycyclohexyl) cyclohexanone
$C_{12}H_{20}O_6$	139-45-7	45-092	1,2,3-Propanetriyl tripropanoate	1,2,3-Propanetriyl ester propanoic acid; Tripropionin
$C_{12}H_{22}$	92-51-3	12-065 /B+S2	1,1′-Bicyclohexyl	Cyclohexylcyclohexane; Dodecahydrobiphenol
	28777-88-0	12-066	Decahydrodimethylnaphthalene	Dimethyldecalin (unspecified isomer)
	25551-49-9	12-067	Ethyldecahydronaphthalene	Ethyldecalin (unspecified isomer)
	1008-17-9	12-068	1-Ethyldecahydronaphthalene	1-Ethyldecalin; α-Ethyldecalin (unspecified stereoisomer)
	1618-23-1	12-069	2-Ethyldecahydronaphthalene	2-Ethyldecalin; β-Ethyldecalin (unspecified stereoisomer)
	88889-26-3	12-070	Octahydro(1-methylethyl)-1*H*-indene	Hexahydroisopropylindan; Isopropylhydrindan (unspecified isomer)
$C_{12}H_{22}O$	58879-21-3	42-119 /S1	*Trans*-[1,1′-Bicyclohexyl]-2-ol	*Trans*-2-Cyclohexylcyclohexanol
$C_{12}H_{22}O_2$	2664-55-3	45-093	Nonyl 2-propenoate	Nonyl ester 2-propenoic acid; Nonyl acrylate
	2157-01-9	45-094	Octyl 2-methyl-2-propenoate	Octyl ester 2-methyl-2-propenoic acid; Octyl methacrylate
$C_{12}H_{22}O_4$	925-06-4	45-096	Bis(2-methylpropyl) butanedioate	Bis(2-methylpropyl) ester butanedioic acid; Diisobutyl succinate
	2051-00-5	45-095	Bis(3-methylbutyl) ethanedioate	Bis(3-methylbutyl) ester ethanedioic acid; Diisoamyl oxalate
	141-03-7	45-097	Dibutyl butanedioate	Dibutyl ester butanedioic acid; Dibutyl succinate
$C_{12}H_{22}O_4Pb$	15773-53-2	74-004	Lead (2+) salt hexanoic acid	Lead(II) hexanoate; Lead(II) caproate
$C_{12}H_{22}S$	7133-46-2	51-030 /S1+S2	1,1′-Thiobis(cyclohexane)	Dicyclohexyl sulfide
$C_{12}H_{23}BF_4N_2$	244193-52-0	75-034 /S2	1-Methyl-3-octyl-1*H*-imidazolium tetrafluoroborate	[Moim][BF_4][BF_4]; [Omim][BF_4]
$C_{12}H_{23}BrN_2$	61545-99-1	75-035 /S2	1-Methyl-3-octylimidazolium bromide	[Omim][Br]
$C_{12}H_{24}$	294-62-2	12-140 /S2	Cyclododecane	
	112-41-4	13-037	1-Dodecene	α-Dodecylene
$C_{12}H_{24}N_2O_2$	10263-96-4	62-091	*N*,*N*′-Dipropylhexanediamine	*N*,*N*′-Dipropyladipamide
$C_{12}H_{24}O_2$	112-17-4	45-098 /B+S1	Decyl acetate	
	143-7-7	44-027	Dodecanoic acid	Lauric acid
	1731-86-8	45-172 /S2	Methyl undecanoate	Methyl ester undecanoic acid
$C_{12}H_{25}NO$	16238-16-7	62-092	*N*,*N*-Dipentylacetamide	
$C_{12}H_{26}$	112-40-3	11-049 /B+S1+S2	Dodecane	Dihexyl
	13475-82-6	11-050	2,2,4,6,6-Pentamethylheptane	
$C_{12}H_{26}O$	112-53-8	42-095 /B+S1+S2	1-Dodecanol	Dodecyl alcohol; Lauryl alcohol
$C_{12}H_{26}O_3$	112-73-2	41-047 /B+S1	1,1′-[Oxybis(1,2-ethanediyloxy)] bis(butane)	Bis(2-butoxyethyl)ether; Diethylene glycol dibutyl ether
$C_{12}H_{26}O_5$	24800-25-7	47-066 /S1	2-[2-[2-(2-Hydroxypropoxy)propoxy] propoxy]-1-propanol	Tetra(propylene glycol)
$C_{12}H_{26}O_7$	2615-15-8	47-067 /S1	3,6,9,12,15-Pentaoxaheptadecane-1,17-diol	Hexa(ethylene glycol)

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{12}H_{26}S$	6294-31-1	51-024	1,1′-Thiobis(hexane)	7-Thiatridecane; Dihexyl sulfide
$C_{12}H_{27}N$	102-82-9	31-068 /S2	*N*,*N*-Dibutyl-1-butanamine	Tributylamine; Tris(*n*-butylamine)
$C_{12}H_{27}O_4P$	126-73-8	72-018 /S1	Tributyl ester phosphoric acid	Tributyl phosphate
$C_{12}H_{28}O_4Si$	682-01-9	71-034	Tetrapropyl ester silicic acid	Tetrapropyl orthosilicate; Tetrapropoxysilane
$C_{12}H_{30}OSi_2$	994-49-0	71-035	Hexaethyldisiloxane	
$C_{12}H_{30}O_3Si_3$	2031-79-0	71-036	Hexaethylcyclotrisiloxane	
$C_{13}H_9F_3N_2O_2$	4394-00-7	64-040 /S1	2-[[3-(Trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	Niflumic acid
$C_{13}H_9N$	260-94-6	33-042	Acridine	Benzo[*b*]quinoline; 2,3,5,6-Dibenzopyridine
	230-27-3	33-043	Benzo[*h*]quinoline	7,8-Benzoquinoline
	229-87-8	33-044	Phenanthridine	Benzo[*c*]quinoline
$C_{13}H_{10}$	86-73-7	14-061 /B+S1	9*H*-Fluorene	α-Diphenylenemethane
$C_{13}H_{10}N_2$	622-16-2	34-013	*N*,*N*′-Methanetetraylbis(benzenamine)	Diphenylcarbodiimide
$C_{13}H_{10}O$	119-61-9	43-051 /B+S2	Diphenyl methanone	Diphenyl ketone; Benzophenone
$C_{13}H_{10}O_3$	118-55-8	47-041 /B+S2	Phenyl ester 2-hydroxybenzoic acid	Phenyl salicylate; Salol
$C_{13}H_{11}Cl$	90-99-3	22-048	1,1′-(Chloromethylene)bis(benzene)	Diphenylchloromethane
$C_{13}H_{11}N$	1484-12-4	33-045	9-Methyl-9*H*-carbazole	
$C_{13}H_{12}$	101-81-5	14-062 /B+ S2	1,1′-Methylenebis(benzene)	Diphenylmethane; Benzylbenzene
$C_{13}H_{13}N$	552-82-9	31-043	*N*-Methyl-*N*-phenylbenzenamine	*N*-Methyldiphenylamine
$C_{13}H_{14}N_2$	101-77-9	31-044	4,4′-Methylenebis(benzenamine)	4,4′-Methylenedianiline; Bis(4-aminophenyl)methane
$C_{13}H_{15}Cl_2N_3$	66246-88-6	64-047 /S2	1-[2-(2,4-Dichlorophenyl)pentyl-1*H*-1,2,4-triazole	Penconazole
$C_{13}H_{15}N$	6303-88-4	33-046	2,3,4,9-Tetrahydro-9-methyl-1*H*-carbazole	1,2,3,4-Tetrahydro-9-methylcarbazole
$C_{13}H_{15}NO$	2094-99-7	62-093	1-(1-Isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene	*m*-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
	2889-58-9	62-094	1-(1-Isocyanato-1-methylethyl)-4-(1-methylethenyl)benzene	*p*-Isopropenyl-α,α-dimethylbenzyl ester isocyanic acid
$C_{13}H_{17}FeN$	1271-86-9	73-058 /S2	[(Dimethylamino)methyl]ferrocene	(Ferrocenylmethyl) dimethylamine
$C_{13}H_{18}$	941-60-6	14-063	1,1,4,6-Tetramethylindan	
	1078-04-2	14-064	1,1,4,7-Tetramethylindan	
$C_{13}H_{18}F_6N_2O_4S_2$	460983-97-5	75-036 /S2	1-Hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Hpy][Tf2N]
$C_{13}H_{18}O_2$	15687-27-1	44-046 /S2	*a*-Methyl-4-(2-methylpropyl)benzeneacetic acid	(*R*,*S*)-Ibuprofen; 2-(4-Isobutylphenyl)propionic acid
$C_{13}H_{19}F_6N_3O_4S_2$	900797-79-7	75-037 /S2	1-Butyl-4-dimethylaminopyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[BAPY][BTI]
$C_{13}H_{19}NO_2$	7461-26-9	62-095	Hexyl ester phenylcarbamic acid	Hexyl phenylcarbamate; Hexyl ester carbanilic acid
$C_{13}H_{20}$	1078-71-3	14-065 /B+S2	Heptylbenzene	1-Phenylheptane
$C_{13}H_{20}O$	141-10-6	43-052	6,10-Dimethyl-3,5,9-undecatriene-2-one	Pseudoionone; Ψ-Ionone
	16647-05-5	43-053	6,10-Dimethyl-4,5,9-undecatriene-2-one	
	14901-07-6	43-054	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	β-Ionone
$C_{13}H_{21}F_6N_3O_4S_2$	384347-22-2	75-038 /S2	1-Hexyl-2,3-dimethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Hmmim][Tf2N]
$C_{13}H_{22}$	707-35-7	12-071 /B+S2	1,3,5-Trimethyltricyclo [3.3.1.1^{3,7}] decane	1,3,5-Trimethyladamantane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{13}H_{23}F_3N_2O_3S$	403842-84-2	75-039 /S2	1-Octyl-3-methylimidazolium trifluoromethanesulfonate	[Omim][OTf]
$C_{13}H_{24}$	27193-29-9	12-072	Decahydro(1-methylethyl)naphthalene	Isopropyldecalin (unspecified isomer)
	1010-74-8	12-073	Decahydro-1-(1-methylethyl)naphthalene	Decahydro-1-isopropylnaphthalene; α-Isopropyldecalin
	91972-45-1	12-074	Decahydro-1-propylnaphthalene	1-Propyldecalin; α-Propyldecalin
	999999-0-5	12-075	2-Methyl-1,1′-bicyclohexyl	1-Methylcyclohexylcyclohexane
	3178-23-2	12-076	1,1′-Methylenebis(cyclohexane)	Dicyclohexylmethane
$C_{13}H_{24}O_2$	2696-43-7	45-099	Nonyl 2-methyl-2-propenoate	Nonyl ester 2-methyl-2-propenoic acid; Nonyl methacrylate
	1725-04-8	47-042	Oxacyclotetradecan-2-one	Tridecanolide; Tridecanolactone
$C_{13}H_{25}NO_3$	95639-17-1	62-169 /S1	α-[(Cyclohexyloxy)methyl]-4-morpholineethanol	1-Morpholino-3-cyclohexyloxy-2-propanol
$C_{13}H_{26}$	5617-41-4	12-077	Heptylcyclohexane	
$C_{13}H_{26}N_2O_6S$	595565-54-1	75-040 /S2	1-Butyl-3-methyl-1*H*-imidazolium 2-(2-methoxyethoxy)ethyl sulfate	
$C_{13}H_{26}O$	1604-34-8	43-055	6,10-Dimethyl-2-undecanone	Hexahydropseudoionone
$C_{13}H_{26}O_2$	627-90-7	45-173 /S2	Ethyl undecanoate	Ethyl ester undecanoic acid
	111-82-0	45-174 /S2	Methyl dodecanoate	Methyl laurate; Methyl laurinate
	638-53-9	44-028	Tridecanoic acid	Tridecylic acid
	1731-81-3	45-143 /S1	Undecyl acetate	
$C_{13}H_{26}O_2Si_3$	546-44-1	71-037	1,1,1,3,5,5,5-Heptamethyl-3-phenyltrisiloxane	
$C_{13}H_{28}$	629-50-5	11-051 /B+S2	Tridecane	
$C_{13}H_{28}O$	597-93-3	42-096	5-Butyl-5-nonanol	
	112-70-9	42-097 /B+S1+S2	1-Tridecanol	*n*-Tridecyl alcohol
$C_{14}F_{30}$	307-62-0	21-053 /S1	Triacontafluorotetradecane	Perfluorotetradecane
$C_{14}H_8Fe$	31904-29-7	73-059 /S2	Butylferrocene	Butylcyclopentadienyl (cyclopentadienyl)iron
$C_{14}H_8O_2$	84-65-1	43-056	9,10-Anthracenedione	9,10-Antraquinone
$C_{14}H_{10}$	120-12-7	14-066 /B+S1+S2	Anthracene	
	501-65-5	14-067 /B+ S2	1,1′-(1,2-Ethynediyl)bis(benzene)	1,2-Diphenylacetylene; Tolan
	85-01-8	14-068 /B+S1+S2	Phenanthrene	
$C_{14}H_{12}$	103-30-0	14-070	(*E*)-1,1′-(1,2-Ethenediyl)bis(benzene)	*Trans*-1,2-Diphenylethylene; Stilbene; Toluylene
	613-31-0	14-112 /S1	9,10-Dihydroanthracene	
	776-35-2	14-069	9,10-Dihydrophenanthrene	
	530-48-3	14-071 /B+S1	1,1′-Ethenylidenebis(benzene)	1,1-Diphenylethylene
$C_{14}H_{12}O$	24324-17-2	42-135 /S2	9*H*-Fluorene-9-methanol	9-Fluorenylmethanol
	643-65-2	43-057	(3-Methylphenyl)phenylmethanone	3-Methylbenzophenone; Phenyl *m*-tolyl ketone
$C_{14}H_{12}O_4$	840-65-3	45-144 /S1	Dimethyl ester 2,6-naphthalenedicarboxylic acid	
$C_{14}H_{14}$	605-39-0	14-113 /S1	2,2′-Dimethyl-1,1′-biphenyl	2,2′-Dimethylbiphenyl
	103-29-7	14-072	1,1′-(1,2-Ethanediyl)bis(benzene)	Bibenzyl; 1,2-Diphenylethane; *sym*-Diphenylethane; Dibenzyl
	1812-51-7	14-114 /S1	2-Ethyl-1,1′-biphenyl	2-Ethylbiphenyl
	612-00-0	14-073 /B+S1	1,1′-Ethylidenebis(benzene)	1,1-Diphenylethane; *unsym*-Diphenylethane
	713-36-0	14-115 /S1	1-Methyl-2-(phenylmethyl)benzene	Phenyl-*o*-tolylmethane
	2141-42-6	14-116 /S1	1,2,3,4-Tetrahydroanthracene	
	1013-08-7	14-117 /S1	1,2,3,4-Tetrahydrophenanthrene	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{14}H_{14}N_2O_3$	1562-94-3	62-096	Bis(4-methoxyphenyl)diazene-1-oxide	4,4′-Dimethoxyazoxybenzene; *p*-Azoxyanisole
$C_{14}H_{14}O$	103-50-4	41-050 /S1	1,1′-[Oxybis(methylene)]bis(benzene)	Dibenzyl ether
$C_{14}H_{16}$	17872-39-8	12-131 /S1	Dodecahydro-1,3,4,6-ethanediylidenedi cyclopenta[*cd*,*gh*]pentalene	Heptacyclo [6.6.0^{2,6}.0^{3,13}.0^{4,11}.0^{5,9}.0^{10,14}] tetradecane
$C_{14}H_{16}N_2O_2$	2778-42-9	62-097	1,3-Bis(1-isocyanato-1-methylethyl)benzene	$\alpha,\alpha,\alpha',\alpha'$-Tetramethyl-*m*-xylylene ester isocyanic acid
	2778-41-8	62-098	1,4-Bis(1-isocyanato-1-methylethyl)benzene	$\alpha,\alpha,\alpha',\alpha'$-Tetramethyl-p-xylylene ester isocyanic acid
$C_{14}H_{18}$	66289-74-5	12-132 /S1	Dodecahydro-4,7-methano-2,3,8-methe nocyclopent[*a*]indene (stereoisomer HNN)	Hexacyclic *endo*,*endo*-dihydrodinorbornadiene
	66289-73-4	12-133 /S1	Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXN)	Hexacyclic *exo*,*endo*-dihydronorbornadiene
	64162-49-8	12-134 /S1	Dodecahydro-4,7-methano-2,3,8-methenocyclopent[*a*]indene (stereoisomer HXX)	Hexacyclic *exo*,*exo*-dihydrodinorbornadiene
	1079-71-6	14-074	1,2,3,4,5,6,7,8-Octahydroanthracene	
$C_{14}H_{20}$	2292-79-7	12-078	Decahydro-3,5,1,7-[1,2,3,4] butanetetraylnaphthalene	Diamantane
	25079-41-8	12-135 /S1	Dodecahydro-1,4:5,8-dimethanobiphenylene	Pentacyclic *exo*,*transexo*-tetrahydrodinorbornadiene
$C_{14}H_{20}F_6N_2O_4S_2$	547718-92-3	75-041 /S2	1-Hexyl-3-methylpyridinium 1,1,1-trifluoro-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Hmpy][Tf2N]
$C_{14}H_{20}O_3$	64533-95-5	47-043	1-[4-(1,1-Diethoxyethyl)phenyl]ethanone	*p*-Diacetylbenzene diethyl ketal
$C_{14}H_{22}$	1012-72-2	14-130 /S2	1,4-Bis(1,1-dimethylethyl)benzene	1,4-Di-*tert*-butylbenzene
	2189-60-8	14-075	Octylbenzene	1-Phenyloctane
$C_{14}H_{22}N_2O$	14585-29-6	62-170 /S1	1-Anilino-3-piperidino-2-propanol	
$C_{14}H_{23}F_6N_3O_4S_2$	178631-04-4	75-042 /S2	1-Methyl-3-octy-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide	[Moim][Tf2N]; [Omim][Tf2N]
$C_{14}H_{23}NO_2$	3578-07-2	62-171 /S1	Decyl ester 2-cyano-2-propenoic acid	*n*-Decyl α-cyanacrylate
$C_{14}H_{24}$	92431-75-9	12-079	Dodecahydro-9-methylfluorene	9-Methylperhydrofluorene
	5743-97-5	12-080 /B+S1	Tetradecahydrophenanthrene	Perhydrophenanthrene; Tricyclo [8.4.0.0^{2,7}] tetradecane (mixture of stereoisomers)
	27425-35-0	12-081	(4aα,4bα,8aα,10aβ)-Tetradecahydrophenanthrene	*cis-syn-trans*-Perhydrophenantrene
	27389-73-7	12-082	(4aα,4bβ,8aα,10aα)-Tetradecahydrophe nanthrene	*trans-anti-cis*-Perhydrophenanthrene
	2108-89-6	12-083	(4aα,4bβ,8aα,10aβ)-Tetradecahydrophe nanthrene	*trans-anti-trans*-Perhydrophenanthrene
$C_{14}H_{26}$	92369-80-7	12-084	1-Butyldecahydronaphthalene	1-Butyldecalin; α-Butyldecalin
	66826-96-8	12-085	1-(Cyclohexylmethyl)-2-methylcyclohexane	Cyclohexyl(2-methylcyclohexyl) methane
	92369-82-9	12-086	Decahydro-1-(1-methylpropyl)naphthalene	1-*sec*-Butyldecahydronaphthalene; α-*sec*-Butyldecalin
	92369-83-0	12-087	Decahydro-1-(2-methylpropyl)naphthalene	Decahydro-1-isobutylnaphthalene; α-Isobutyldecalin
	27193-30-2	12-088	(1,1-Dimethylethyl)decahydronaphthalene	*tert*-Butyldecalin (unspecified isomer)
	3321-50-4	12-089	1,1′-(1,2-Ethanediyl)bis(cyclohexane)	1,2-Dicyclohexylethane
	66826-94-6	12-090	2-Ethyl-1,1′-bicyclohexyl	2-Ethylcyclohexylcyclohexane
	2319-61-1	12-091	1,1′-Ethylidenebis(cyclohexane)	1,1-Dicyclohexylethane
$C_{14}H_{26}O$	99914-84-8	43-058	2-(1,2-Dimethylpropyl)-5,6-dimethyl-2-heptenal	
	3021-89-4	43-059	2-Pentyl-2-nonenal	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{14}H_{26}O_2$	3179-47-3	45-100	Decyl 2-methyl-2-propenoate	Decyl ester 2-methyl-2-propenoic acid; Decyl methacrylate
$C_{14}H_{26}O_4$	818-04-2	45-101	Bis(3-methylbutyl) butanedioate	Bis(3-methylbutyl) ester butanedioic acid; Diisoamyl succinate
	105-99-7	45-145 /S1	Dibutyl ester hexanedioic acid	Dibutyl adipate
$C_{14}H_{26}O_4Pb$	16180-10-2	74-028 /S1	Lead (2+) salt heptanoic acid	Lead(II) heptanoate; Lead(II) oenanthate
$C_{14}H_{27}NO_2$	96450-92-9	62-172 /S1	α-[(Cyclohexyloxy)methyl]-1-piperidineethanol	1-Piperidino-3-cyclohexoxy-2-propanol
$C_{14}H_{28}O$	2345-27-9	43-060	2-Tetradecanone	Dodecyl methyl ketone
$C_{14}H_{28}O_2$	112-66-3	45-146 /S1	Dodecyl acetate	
	1731-88-0	45-175 /S2	Methyl tridecanoate	Methyl ester tridecanoic acid
	544-63-8	44-029	Tetradecanoic acid	Myristic acid
$C_{14}H_{30}$	629-59-4	11-052 /B+S1+S2	Tetradecane	
$C_{14}H_{30}O$	112-72-1	42-098 /B+S1	1-Tetradecanol	*n*-Tetradecyl alcohol; Myristyl alcohol
$C_{14}H_{30}O_5$	39619-69-7	47-084 /S2	3,6,9,12-Tetraoxadecan-1-ol	Tetraethylene glycol hexyl ether
$C_{14}H_{30}S$	629-65-2	51-025	1,1′-Thiobis(heptane)	8-Thiapentadecane; Diheptyl sulfide
$C_{15}H_{10}N_2O_2$	101-68-8	62-099 /B+S1	1,1′-Methylenebis(4-isocyanatobenzene)	Methylenedi-*p*-phenylene ester isocyanic acid; Diphenylmethane-4,4′-diisocyanate
$C_{15}H_{12}$	832-64-4	14-076	4-Methylphenanthrene	
$C_{15}H_{14}F_2$	137528-87-1	21-057 /S2	3,5-Difluoro-4′-propyl-1,1′-biphenyl	2,6-Difluoro-4-(4-propylphenyl)benzene
$C_{15}H_{16}$	25640-78-2	14-077	(1-Methylethyl)-1,1′-biphenyl	Isopropylbiphenyl; Isopropyldiphenyl (unspecified isomer)
	1081-75-0	14-118 /S1	1,1′-(1,3-Propanediyl)bis(benzene)	1,3-Diphenylpropane
$C_{15}H_{16}N_2O_3$	56095-14-8	62-100	(4-Ethoxyphenyl)(4-methoxyphenyl)diazene-*N*-oxide	4-Ethoxy-4′-methoxyazoxybenzene; *p*-Azoxyanisoylphenetole
$C_{15}H_{16}O_2$	80-05-7	42-099	4,4′-(1-Methylethylidene)bis(phenol)	4,4′-Isopropylidenediphenol; 4,4′-Dihydroxydiphenyl-2,2-propane
$C_{15}H_{16}S_2$	14252-46-1	51-031 /S1	1,1′-[(1-Methylethylidene)bis(thio)] bis(benzene)	2,2′-Bis(phenylthio)propane
$C_{15}H_{22}F_6N_2O_4S_2$	872672-54-3	75-043 /S2	1-Hexyl-3,5-dimethylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Hmmpy][Tf2N]
$C_{15}H_{23}F_6N_3O_4S_2$	872672-57-6	75-044 /S2	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[hDMApy][Tf2N]; [HAPY][BTI]
$C_{15}H_{24}$	717-74-8	14-119 /S1	1,3,5-Tris(1-methylethyl)benzene	1,3,5-Triisopropylbenzene
$C_{15}H_{26}$	6051-40-7	12-092	1,1′:3′,1″-Tercyclopentane	1,3-Dicyclopentylcyclopentane
$C_{15}H_{26}O_6$	60-01-5	45-102	1,2,3-Propanetriyl tributanoate	1,2,3-Propanetriyl ester butanoic acid; Tributyrin
$C_{15}H_{28}$	97239-02-6	12-093	Cyclohexyl(ethylcyclohexyl)methane (unspecified isomer)	
	66374-71-8	12-094	1-(Cyclohexylmethyl)-2-ethylcyclohexane	Cyclohexyl(2-ethylcyclohexyl) methane
	41851-34-7	12-095	1,2-Dicyclohexylpropane	
	31624-59-6	12-096	(1-Methylethyl)-1,1′-bicyclohexyl	Isopropylbicyclohexyl; Isopropylcyclohexylcyclohexane (unspecified isomer and stereoisomer)
$C_{15}H_{28}O$	1604-35-9	42-100	3,7,11-Trimethyl-1-dodecyn-3-ol	
$C_{15}H_{28}O_2$	106-02-5	47-044	Oxacyclohexadecan-2-one	Pentadecanolide; Pentadecanolactone; 15-Hydroxypentadecanoic acid lactone
$C_{15}H_{30}$	1795-21-7	12-097	Decylcyclopentane	Cyclopentyldecane
$C_{15}H_{30}InN_3S_6$	15741-07-8	73-044 /S1	Tri(diethylcarbamodithioato-*S*,*S*′)indium	
$C_{15}H_{30}O$	2345-28-0	43-061	2-Pentadecanone	Methyl tridecyl ketone

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{15}H_{30}O_2$	28267-29-0	45-176 /S2	Ethyl tridecanoate	Ethyl ester tridecanoic acid
	124-10-7	45-103 /B+S2	Methyl tetradecanoate	Methyl myristate
	1002-84-2	44-030	Pentadecanoic acid	Pentadecylic acid
$C_{15}H_{32}$	629-62-9	11-053 /B+S2	Pentadecane	
$C_{15}H_{32}O$	629-76-5	42-101 /B+S2	1-Pentadecanol	*n*-Pentadecyl alcohol
$C_{15}H_{32}O_6$	21482-12-2	47-068 /S1	2,5,8,11-Tetramethyl-3,6,9,12-tetraoxapentadecane-1,14-diol	Penta(propylene glycol)
$C_{16}F_{34}$	355-49-7	21-054 /S1	Tetratriacontafluorohexadecane	Perfluorohexadecane
$C_{16}H_{10}$	206-44-0	14-078 /B+S1	Fluoranthene	
	129-00-0	14-079 /B+S1+S2	Pyrene	
$C_{16}H_{12}Ge$	1675-59-8	73-030	Diethynyldiphenylgermane	
$C_{16}H_{12}Si$	1675-57-6	71-038	Diethynyldiphenylsilane	
$C_{16}H_{14}$	781-17-9	14-120 /S1	4,5,9,10-Tetrahydropyrene	
$C_{16}H_{14}N_2$	19311-79-6	33-060 /S2	1-Methyl-3,5-diphenyl-1*H*-pyrazole	
$C_{16}H_{14}O_2$	495-71-6	43-062	1,4-Diphenyl-1,4-butanedione	1,2-Dibenzoylethane
$C_{16}H_{15}N$	58743-76-3	32-029 /S1	4′-Propyl[1,1′-biphenyl]-4-carbonitrile	4′-Propylbiphenyl-4-carbonitrile
$C_{16}H_{16}$	1732-13-4	14-121 /S1	1,2,3,6,7,8-Hexahydropyrene	
$C_{16}H_{16}N_2O_2$	2299-73-2	62-101	[(4-Methoxyphenyl)methylene] hydrazone-4-methoxybenzaldehyde	*p*-Anisaldehydeazine; Anisaldazine
$C_{16}H_{18}$	1634-11-3	14-122 /S1	1,1′-(2-Methylpropylidene)bis(benzene)	2-Methyl-1,1-diphenylpropane
$C_{16}H_{18}N_2O_3$	4792-83-0	62-102	Bis(4-ethoxyphenyl)diazene-1-oxide	4,4′-Diethoxyazoxybenzene; *p*-Azoxyphenetole
$C_{16}H_{20}Cr$	12212-68-9	73-045 /S1	Bis[(1,2,3,4,5,6-η)-ethylbenzene] chromium	Bis(ethylbenzene)chromium
$C_{16}H_{21}N$	61203-99-4	32-031 /S2	4-(*trans*-4-Propylcyclohexyl)benzonitrile	*trans*-4-Propyl-1-(4-cyanophenyl) cyclohexane
$C_{16}H_{22}F_6N_2O_6S_2$	872672-53-2	75-045 /S2	3-(Butoxycarbonyl)-1-butylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[b2Nic][Tf2N]
$C_{16}H_{22}OSi_2$	56-33-7	71-039 /B+S1	1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane	
$C_{16}H_{22}O_3Si_3$	1693-51-2	71-040	2,2,4,4-Tetramethyl-6,6-diphenylcyclotrisiloxane	
$C_{16}H_{22}O_4$	84-74-2	45-104 /B+S1+S2	Dibutyl 1,2-benzenedicarboxylate	Dibutyl ester 1,2-benzenedicarboxylic acid; Dibutyl phthalate
$C_{16}H_{24}F_6N_2O_4S_2$	712355-02-7	75-046 /S2	3-Methyl-1-octylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Ompy][Tf2N]
$C_{16}H_{25}F_6N_3O_4S_2$	872672-59-8	75-047 /S2	4-(Dimethylamino)-1-hexyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[hmDMApy][TfN]
$C_{16}H_{25}NO_2$	33689-71-3	62-103	Nonyl phenylcarbamate	Nonyl ester phenylcarbamic acid; Nonyl ester carbanilic acid
$C_{16}H_{27}N$	65355-35-3	32-030 /S1	[*trans*(*trans*)]-4′-Propyl-[1,1′-bicyclohexyl]-4-carbonitrile	*trans*,*trans*-4′-Propylbicyclohexyl-4-carbonitrile
$C_{16}H_{28}$	2320-05-0	12-098	1-Cyclohexyloctahydro-3-methyl-1*H*-indene	1-Cyclohexyl-3-methylhydrindan
	90591-84-7	12-099	2-Ethyltetradecahydrophenanthrene	2-Ethylperhydrophenanthrene
$C_{16}H_{30}$	97676-41-0	12-101	Cyclohexyl[(1-methylethyl)cyclohexyl] methane	Cyclohexyl(isopropylcyclohexyl) methane (unspecified isomer)
	41851-35-8	12-100	1,1′-(1-Methyl-1,3-propanediyl)bis (cyclohexane)	1,3-Dicyclohexylbutane
$C_{16}H_{30}HgO_4$	28043-54-1	74-005	Mercury (2+) salt octanoic acid	Mercury(II) octanoate; Mercury(II) caprylate
$C_{16}H_{30}O_4Pb$	7319-86-0	74-006	Lead (2+) salt octanoic acid	Lead(II) octanoate; Lead(II) caprylate
$C_{16}H_{32}$	1795-16-0	12-102	Decylcyclohexane	Cyclohexyldecane

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	629-73-2	13-038	1-Hexadecene	α-Hexadecylene; Cetene
$C_{16}H_{32}O_2$	57-10-3	44-031 /B+S1	Hexadecanoic acid	Palmitic acid
	7132-64-1	45-177 /S2	Methyl pentadecanoate	
	638-59-5	45-147 /S1	Tetradecyl acetate	
$C_{16}H_{33}Cl$	4860-03-1	22-068 /S2	1-Chlorohexadecane	1-Hexadecyl chloride; Cetyl chloride
$C_{16}H_{34}$	4390-04-9	11-054 /B+S1	2,2,4,4,6,8,8-Heptamethylnonane	
	544-76-3	11-055 /B+S1+S2	Hexadecane	Cetane
$C_{16}H_{34}O$	36653-82-4	42-102 /B+S1+S2	1-Hexadecanol	Hexadecyl alcohol; Cetyl alcohol
	629-82-3	41-051 /S1	1,1′-Oxybis(octane)	Dioctyl ether
$C_{16}H_{34}O_6$	86674-95-5	47-085 /S2	3,6,9,12,15-Pentaoxaheneicosan-1-ol	Pentaethylene glycol hexyl ether
$C_{16}H_{34}S$	2690-08-6	51-026 /B+S1	1,1′-Thiobis(octane)	9-Thiaheptadecane; Dioctyl sulfide
$C_{16}H_{35}N$	99916-30-0	31-045	*N*,*N*-Dimethyl-2-pentyl-1-nonanamine	*N*,*N*-Dimethyl-2-pentylnonylamine
	1120-48-5	31-064 /S1	*N*-Octyl-1-octanamine	*N*,*N*-Dioctylamine
$C_{16}H_{36}Ge$	1067-42-1	73-031	Tetrabutylgermane	
$C_{16}H_{36}O_3Si_2$	349140-64-3	71-069 /S2	Methyl ester 11-(1,1,3,3-tetramethyldisiloxanyl) undecanoic acid	
$C_{16}H_{36}O_4Si$	4766-57-8	71-041	Tetrabutyl ester silicic acid	Tetrabutyl orthosilicate; Tetrabutoxysilane
$C_{16}H_{36}O_4Ti$	5593-70-4	74-007	Titanium (4+) salt 1-butanol	Tetrabutoxytitanium
$C_{16}H_{40}O_4Si_4$	1451-99-6	71-042	Octaethylcyclotetrasiloxane	
$C_{17}H_{14}N_2O_2$	1156-51-0	62-173 /S1	(1-Methylethylidene)di-1,4-phenylene ester cyanic acid	2,2-Bis(4-cyanatophenyl)propane
$C_{17}H_{30}$	26447-22-3	12-103	Cyclopentylbicyclohexyl (unspecified isomer)	
$C_{17}H_{32}$	98028-64-9	12-104	Bis(ethylcyclohexyl)methane (unspecified isomer)	
	26637-18-3	12-105	1-Cyclohexyl-1-(1-methylethyl) cyclohexylethane	1-Cyclohexyl-1-(isopropylcyclohexyl) ethane (unspec. isomer)
$C_{17}H_{34}O_2$	506-12-7	44-032	Heptadecanoic acid	Margaric acid
	112-39-0	45-178 /S2	Methyl hexadecanoate	Methyl palmitate
	110-27-0	45-148 /S1	1-Methylethyl ester tetradecanoic acid	Isopropyl myristate
$C_{17}H_{36}$	629-78-7	11-056 /B+S1+S2	Heptadecane	
$C_{17}H_{36}O$	1454-85-9	42-136 /S2	1-Heptadecanol	Heptadecyl alcohol
$C_{18}HF_{15}Ge$	42371-50-6	73-046 /S1	Tris(2,3,4,5,6-pentafluorophenyl) germane	Tri(pentafluorophenyl)germane
$C_{18}H_{12}$	217-59-4	14-080	Triphenylene	9,10-Benzophenanthrene
$C_{18}H_{14}$	84-15-1	14-081	1,1′:2′,1″-Terphenyl	*o*-Terphenyl
	92-06-8	14-082	1,1′:3′,1″-Terphenyl	*m*-Terphenyl
	92-94-4	14-083 /B+S1	1,1′:4′,1″-Terphenyl	*p*-Terphenyl
$C_{18}H_{15}ClSi$	76-86-8	71-044	Chlorotriphenylsilane	
$C_{18}H_{15}OP$	791-28-6	72-012	Triphenylphosphine oxide	Oxotriphenylphosphorane; Oxotriphenylphosphorus
$C_{18}H_{15}O_4P$	115-86-6	72-013	Triphenyl ester phosphoric acid	Triphenyl phosphate
$C_{18}H_{18}$	483-65-8	14-084	1-Methyl-7-(1-methylethyl)phenanthrene	7-Isopropyl-1-methylphenanthrene; Retene
$C_{18}H_{18}N_2O_5$	6421-04-1	62-104	Diethyl ester 4,4′-azoxybis(benzoic acid)	Diethyl 4,4′-azoxybis(benzoate); Ethyl-*p*,*p*-azoxybenzoate
$C_{18}H_{21}NO$	26227-73-6	62-105	4-Butyl-*N*-[(4-methoxyphenyl) methylene]benzenamine	*N*-(*p*-Methoxybenzylidene)-*p*-butylaniline; MBBA
$C_{18}H_{21}NO_2$	52218-22-1	62-106	2-[[(4-Butylphenyl)imino]methyl]-4-methoxyphenol	*N*-(*o*-Hydroxy-*p*-methoxybenzylidene-*p*-butylaniline; 2,4-OHMBBA

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{18}H_{22}$	36876-13-8	14-085	*ar*,*ar*′-Bis(1-methylethyl)-1,1′-biphenyl	Diisopropylbiphenyl (unspecified isomer)
$C_{18}H_{22}N_2O$	98644-12-3	62-107	(*E*)-(4-Butylphenyl)(4-ethoxyphenyl) diazene	
$C_{18}H_{22}N_2O_3$	23315-55-1	62-108	Bis(4-propoxyphenyl)diazene-1-oxide	4,4′-Dipropoxyazoxybenzene
$C_{18}H_{28}O_2Si_3$	797-7-3	71-045	1,1,1,5,5,5-Hexamethyl-3,3-diphenyltri siloxane	
$C_{18}H_{28}O_4Si_4$	30026-85-8	71-046	2,2,4,4,6,6-Hexamethyl-8,8-diphenylcy clotetrasiloxane	
$C_{18}H_{30}$	123-01-3	14-123 /S1	Dodecylbenzene	1-Phenyldodecane
	94262-24-5	12-106	3-Ethylhexadecahydropyrene	3-Ethylperhydropyrene
	635-11-0	14-131 /S2	1,2,4,5-Tetrakis(1-methylethyl)benzene	1,2,4,5-Tetraisopropylbenzene
$C_{18}H_{30}O_4$	47189-08-2	41-048	1,4-Bis(1,1-diethoxyethyl)benzene	*p*-Diacetylbenzene tetraethyl ketal; Ethylacetal *p*-diacetyl benzene
$C_{18}H_{32}$	22236-61-9	12-107	1-Cyclohexyloctahydro-1,3,3-trimethyl-1*H*-indene	1-Cyclohexyl-1,3,3-trimethylhydrindan
	2456-43-1	12-108	1,1′:2′,1″-Tercyclohexane	*o*-Tercyclohexane
	1706-50-9	12-109	1,1′:3′,1″-Tercyclohexane	*m*-Tercyclohexane
	1795-19-3	12-110	1,1′:4′,1″-Tercyclohexane	*p*-Tercyclohexane
$C_{18}H_{32}O$	1604-32-6	43-063	6,10,14-Trimethyl-3,5-pentadecadien-2-one	
$C_{18}H_{34}$	98803-06-6	12-112	1,1,-Bis(dimethylcyclohexyl)ethane (unspecified isomer)	
	98803-07-7	12-111	1,1-Bis(ethylcyclohexyl)ethane (unspecified isomer)	
$C_{18}H_{34}O_2$	112-80-1	44-033 /B+S1	(*Z*)-9-Octadecenoic acid	Oleic acid
$C_{18}H_{34}O_4$	109-43-3	45-105	Dibutyl decanedioate	Dibutyl ester decanedioic acid; Dibutyl sebacate
$C_{18}H_{34}O_4Pb$	63400-08-8	74-029 /S1	Lead (2+) salt nonanoic acid	Lead(II) nonanoate; Lead(II) pelargonate
$C_{18}H_{36}$	1795-17-1	12-113	Dodecylcyclohexane	Cyclohexyldodecane
	98803-61-3	12-114	Hexaethylcyclohexane (unspecified isomer)	
$C_{18}H_{36}N_2O_2$	21150-82-3	62-109	*N*,*N*′-Dihexylhexanediamide	*N*,*N*′-Dihexyladipamide
$C_{18}H_{36}O$	143-28-2	42-120 /S1	(*Z*)-9-Octadecen-1-ol	Oleyl alcohol
	502-69-2	43-064	6,10,14-Trimethyl-2-pentadecanone	Phytone
$C_{18}H_{36}O_2$	1731-92-6	45-179 /S2	Methyl heptadecanoate	Methyl margarate
	57-11-4	44-034 /B+S1	Octadecanoic acid	Stearic acid
$C_{18}H_{37}Cl$	3386-33-2	22-049	1-Chlorooctadecane	
$C_{18}H_{38}$	593-45-3	11-057 /B+S1+S2	Octadecane	
$C_{18}H_{38}O$	112-92-5	42-103 /B+S1+S2	1-Octadecanol	Octadecyl alcohol; Stearyl alcohol
$C_{18}H_{38}O_7$	74388-92-4	47-069 /S1	2,5,8,11,14-Pentamethyl-3,6,9,12,15-pentaoxaoctadecane	Hexa(propylene glycol)
$C_{18}H_{38}S$	929-98-6	51-027	1,1′-Thiobis(nonane)	10-Thianonadecane; Dinonyl sulphide
$C_{18}H_{39}N$	102-86-3	31-069 /S2	*N*,*N*-Dihexyl-1-hexanamine	Trihexylamine; Tri-*n*-hexylamine
$C_{19}H_{15}Cl$	76-83-5	22-064 /S1	1,1′,1″-(Chloromethylidene)tris (benzene)	Triphenylchloromethane
$C_{19}H_{16}$	519-73-3	14-086	1,1′,1″-Methylidynetris(benzene)	Triphenylmethane; Tritane
$C_{19}H_{18}N_2O_3$	1498-88-0	62-184 /S2	1′,3′-Dihydro-1′,3′,3′-trimethyl-6-nitrospiro[2*H*]-1-benzopyran-2,2′-[2*H*] indole	1,3,3-Trimethyl-6′-nitrospiro [indole-2,2′-benzopyran]
$C_{19}H_{20}F_3N_3O_3$	65847-85-0	64-041 /S1	2-(4-Morpholinyl)ethyl ester 2-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid	Morniflumate
$C_{19}H_{20}O_4$	85-68-7	45-149 /S1+S2	Butyl phenylmethyl ester 1,2-benzenedicarboxylic acid	Benzyl butyl phthalate

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{19}H_{22}ClNO$	5219-48-7	64-029	4-Chloro-*N*-[[4-(hexyloxy)phenyl] methylene]benzenamine	*p*-*n*-Hexyloxybenzylidene-amino-*p*′-chlorobenzene
$C_{19}H_{22}FNO$	56544-26-4	64-030	4-Fluoro-*N*-[[4-(hexyloxy)]methylene] benzenamine	*p*-*n*-Hexyloxybenzylidene-amino-*p*′-fluorobenzene
$C_{19}H_{23}NO$	29743-08-6	62-110	4-Butyl-*N*-[(4-ethoxyphenyl) methylene]benzenamine	*p*-Butyl-*N*-(*p*-ethoxybenzylidene)aniline
	5219-49-8	62-111	*N*-[[4-(Hexyloxy)phenyl]methylene] benzenamine	*p*-*n*-Hexyloxybenzylidene-aniline
$C_{19}H_{36}$	94380-80-0	12-115	Bis(2,4,6-trimethylcyclohexyl)methane	
	96667-88-8	12-116	4-Heptyl-1,1′-bicyclohexyl	4-Heptylcyclohexylcyclohexane
	2090-15-5	12-117	1,1′-Heptylidenebis(cyclohexane)	1,1-Dicyclohexylheptane
$C_{19}H_{38}O_2$	14010-23-2	45-180 /S2	Ethyl heptadecanoate	Ethyl margarate
	112-61-8	45-181 /S2	Methyl octadecanoate	Methyl stearate
	142-91-6	45-150 /S1	1-Methylethyl ester hexadecanoic acid	Isopropyl palmitate
	646-30-0	44-035	Nonadecanoic acid	Nonadecylic acid
$C_{19}H_{40}$	629-92-5	11-058 /B+S1+S2	Nonadecane	
	1921-70-6	11-059	2,6,10,14-Tetramethylpentadecane	Pristane
$C_{19}H_{40}O$	1454-84-8	42-121 /S1	1-Nonadecanol	
$C_{20}F_{42}$	37589-57-4	21-055 /S1	Dotetracontafluoroeicosane	Perfluoroeicosane
$C_{20}H_{12}$	50-32-8	14-124 /S1	Benzo[*a*]pyrene	3,4-Benzopyrene
	198-55-0	14-087 /B+S1	Perylene	
$C_{20}H_{14}$	477-75-8	14-088	9,10-Dihydro-9,10[1′,2′]-benzenoanthracene	Triptycene
$C_{20}H_{16}$	58-72-0	14-132 /S2	1,1′,1″-(1-Ethenyl-2-ylidine)tris (benzene)	Triphenylethene
$C_{20}H_{22}N_2O$	35280-78-5	62-112	4-[[[4-(Hexyloxy)phenyl]methylene] amino]benzonitrile	*p*-*n*-Hexyloxybenzylidene-amino-*p*′-benzonitrile
$C_{20}H_{24}N_2O_3$	97402-83-0	62-113	(*E*)-4-[(4-Methoxyphenyl)azo]phenyl ester heptanoic acid	
$C_{20}H_{25}NO$	25959-51-7	62-114	*N*-[[4-(Hexyloxy)phenyl]methylene]-4-methylbenzenamine	*p*-*n*-Hexyloxybenzylidene-*p*′-toluidine
$C_{20}H_{26}N_2O_3$	17051-01-3	62-115	Bis(4-butoxyphenyl)diazene-1-oxide	4,4′-Dibutoxyazoxybenzene
$C_{20}H_{30}O_3Si_3$	108543-32-4	71-047	2,2,4,4-Tetraethyl-6,6-diphenylcyclo-trisiloxane	
$C_{20}H_{32}F_6N_2O_4S_2$	872672-56-5	75-048 /S2	3,5-Diethyl-1-hexyl-2-propylpyri-dinium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide	[Hpeey][Tf2N]
$C_{20}H_{34}$	26446-93-5	12-118	Diethylhexadecahydropyrene	Diethylperhydropyrene
$C_{20}H_{34}O_5Si_5$	51134-26-0	71-048	Octamethyldiphenylcyclopentasiloxane (unspecified isomer)	
$C_{20}H_{38}HgO_4$	27394-49-6	74-008	Mercury (2+) salt decanoic acid	Mercury(II) decanoate; Mercury(II) caprate
$C_{20}H_{38}O$	29171-23-1	42-104	3,7,11,15-Tetramethyl-1-hexadecyn-3-ol	
$C_{20}H_{38}PbO_4$	15773-52-1	74-009	Lead (2+) salt decanoic acid	Lead(II) decanoate; Lead(II) caprate
$C_{20}H_{40}O$	505-32-8	42-105	3,7,11,15-Tetramethyl-1-hexadecen-3-ol	Isophytol
$C_{20}H_{40}O_2$	506-30-9	44-036	Eicosanoic acid	Icosanic acid; Arachidic acid
	1731-94-8	45-182 /S2	Methyl nonadecanoate	
$C_{20}H_{42}$	112-95-8	11-060 /B+S1	Eicosane	Icosane
$C_{20}H_{42}O$	629-96-9	42-122 /S1+S2	1-Eicosanol	
	5333-42-6	42-123 /S1	2-Octyl-1-dodecanol	9-Hydroxymethylnonadecane
$C_{20}H_{42}O_6$	23244-49-7	47-070 /S1	3,6,9,12,15-Pentaoxapentacosan-1-ol	Pentaoxyethylene glycol decyl ether
$C_{20}H_{42}S$	693-83-4	51-028	1,1′-Thiobis(decane)	11-Thiaheneicosane; 11-Thiahenicosane; Didecyl sulfide

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{20}H_{44}Sn$	3765-65-9	73-032	Tetrapentylstannane	Tetrapentyltin
$C_{21}H_{14}N_2O_4$	13676-54-5	62-116	1,1′-(Methylenedi-4,1-phenylene)bis (1*H*-pyrrole-2,5-dione)	Bis(4-maleic acidimidphenyl)methane
$C_{21}H_{16}$	611-48-3	14-089	1-(2-Naphthalenylmethyl)naphthalene	1,2′-Dinaphthylmethane
$C_{21}H_{21}O_4P$	1330-78-5	72-014	Tris(methylphenyl)ester phosphoric acid	Tricresyl phosphate; Tritolyl phosphate (unspecified isomer)
$C_{21}H_{24}O_3Si_3$	3424-57-5	71-049	(2α,4α,6α)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	*cis*-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
	6138-53-0	71-050	(2α,4α,6β)-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	*trans*-2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane
$C_{21}H_{24}O_4$	1675-54-3	47-045	2,2′-[(1-Methylethylidene)bis(4,1-phenyleneoxymethylene)]bis(oxirane)	
$C_{21}H_{38}$	95135-48-1	12-119	9-(2-Ethylhexyl)dodecahydrofluorene	9-(2-Ethylhexyl)perhydrofluorene
	55682-89-8	12-120	1,1′,1″-(1-Propanyl-2-ylidene)tris (cyclohexane)	1,1,3-Tricyclohexylpropane
$C_{21}H_{38}O_6$	621-70-5	45-106	1,2,3-Propanetriyl ester hexanoic acid	1,2,3-Propanetriyl trihexanoate; Trihexanoin; Tricaproin
$C_{21}H_{40}$	95135-87-8	12-121	4-Nonyl-1,1′-bicyclohexyl	4-Nonylcyclohexylcyclohexane
$C_{21}H_{40}O_4$	41395-83-9	45-151 /S1	1-Methyl-1,2-ethanediyl ester nonanoic acid	Propylene dinonanoate; Propyleneglycol dipelargonate
$C_{21}H_{42}InN_3S_6$	85883-33-6	73-047 /S1	Tris[bis(1-methylethyl)carbamodithio-ato-*S*,*S*′]indium	
	87052-01-5	73-048 /S1	Tris(dipropylcarbamodithiato-*S*,*S*′) indium	
$C_{21}H_{42}O_2$	18281-04-4	45-183 /S2	Ethyl nonadecanoate	Ethyl ester nonadecanoic acid
	1120-28-1	45-184 /S2	Methyl eicosanoate	Methyl arachidate
$C_{21}H_{42}O_4$	123-94-4	47-046	2,3-Dihydroxypropyl ester octadecanoicacid	1-Monostearin
$C_{21}H_{44}$	629-94-7	11-061	Heneicosane	Henicosane
$C_{22}H_{14}$	135-48-8	14-090 /B+S1	Pentacene	2,3,6,7-Dibenzoanthracene
$C_{22}H_{14}O_4$	3363-97-1	43-069 /S1	1,1′-(1,4-Phenylene)bis(2-phenylethane dione)	1,4-Bis(phenylglyoxaloyl) benzene
$C_{22}H_{15}F_7O$	303186-20-1	61-062 /S2	4-[Difluoro(3,4,5-trifluorophenoxy) methyl]-3,5-difluoro-4′-propyl-1,1′-biphenyl	
$C_{22}H_{23}NO_3$	39515-41-8	62-185 /S2	2,2,3,3-Tetramethylcyano(3-phenoxyphenyl)methyl ester cyclopropanecarboxylic acid	Fenpropathrin
$C_{22}H_{24}O_6$	26379-55-5	47-047	*trans*-Bis(4-methoxyphenyl)ester 1,4-cyclohexanedicarboxylic acid	Di(*p*-methoxyphenyl)-*trans*-cyclohexane-1,4-dicarboxylate
$C_{22}H_{29}NO$	29743-10-0	62-117	4-Butyl-*N*-[[4-(pentyloxy)phenyl] methylene]benzenamine	*N*-*p*-*n*-Pentyloxybenzylidene-*p*′-*n*-butylaniline
$C_{22}H_{30}N_2O_3$	19482-05-4	62-118	Bis(4-pentyloxyphenyl)diazene-1-oxide	4,4′-Bis(pentyloxy)azoxybenzene
$C_{22}H_{38}$	1459-09-2	14-133 /S2	Hexadecylbenzene	1-Phenylhexadecane
$C_{22}H_{42}O_4$	103-23-1	45-107 /B+S1	Bis(2-ethylhexyl) hexanedioate	Bis(2-ethylhexyl) adipate; Bis(2-ethylhexyl) ester hexanedioic acid
	2449-10-7	45-108	Dihexyl decanedioate	Dihexyl ester decanedioic acid; Dihexyl sebacate
$C_{22}H_{42}O_4Pb$	63400-07-7	74-030 /S1	Lead (2+) salt undecanoic acid	Lead(II) undecanoate
$C_{22}H_{44}N_2O_2$	31827-03-9	62-119	*N*,*N*′-Dihexyldecanediamine	*N*,*N*′-Dihexylsebacamide
$C_{22}H_{44}O_2$	123-95-5	45-109	Butyl octadecanoate	Butyl ester octadecanoic acid; Butyl stearate
$C_{22}H_{45}Br$	6938-66-5	23-039	1-Bromodocosane	*n*-Docosyl bromide
$C_{22}H_{46}$	629-97-0	11-062	Docosane	
$C_{22}H_{46}O$	661-19-8	42-124 /S1	1-Docosanol	
$C_{22}H_{46}O_6$	3055-95-6	47-071 /S1	3,6,9,12,15-Pentaoxaheptacosan-1-ol	Pentaoxyethylene glycol dodecyl ether
$C_{22}H_{46}O_7$	5168-89-8	47-072 /S1	3,6,9,12,15,18-Hexaoxaoctacosan-1-ol	Hexaoxyethylene glycol decyl ether

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{23}H_{31}NO$	29743-11-1	62-120	4-Butyl-*N*-[[4-(hexyloxy)phenyl] methylene]benzenamine	*N*-*p*-*n*-Hexyloxybenzylidene-*p*′-*n*-butylaniline
$C_{23}H_{44}O_5$	820-17-7	47-048	3-(Acetyloxy)-2-hydroxypropyl ester octadecanoic acid	3-Aceto-1-stearin
$C_{23}H_{46}O_2$	929-77-1	45-185 /S2	Methyl docosanoate	Methyl behenate
$C_{23}H_{48}$	638-67-5	11-063	Tricosane	
$C_{24}F_{50}$	1766-41-2	21-056 /S1	Pentacontafluorotetracosane	Perfluorotetracosane
$C_{24}H_{18}$	612-71-5	14-091	5′-Phenyl-1,1′:3′,1″-terphenyl	1,3,5-Triphenylbenzene
	1166-18-3	14-092	1,1′:3′,1″:3″,1‴-Quaterphenyl	*m*-Quaterphenyl
$C_{24}H_{32}O_3$	38454-35-2	47-049	4-(Heptyloxy)phenyl ester 4-butylbenzoic acid	*p*-(Heptyloxy)phenyl *p*-butylbenzoate
$C_{24}H_{32}O_8$	14174-09-5	46-033 /S2	6,7,9,10,12,13,20,21,23,24,26,27-Dodecahydrodibenz[*b*,*n*][1,4,7,10,13,16,19,22] octaoxacyclotetracosin	Dibenzo-24-crown-8
$C_{24}H_{34}$	1603-53-8	14-093	1,1-Diphenyldodecane	
$C_{24}H_{34}N_2O_3$	2587-42-0	62-121	Bis(4-hexyloxyphenyl)diazene-1-oxide	4,4′-Bis(hexyloxy) azoxybenzene
$C_{24}H_{36}Cr$	38744-20-6	73-049 /S1	Bis[(1,2,3,4,5,6-η)-bis(1-methylethyl) benzene]chromium	Bis(diisopropylbenzene) chromium
$C_{24}H_{37}N_3O_2$	218765-43-6	62-186 /S2	Dodecanoic acid, comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1)	Pyrimenthanil laurate
$C_{24}H_{38}O_4$	117-81-7	45-110 /B+S1+S2	Bis(2-ethylhexyl)-1,2-benzenedi-carboxylate	Bis(2-ethylhexyl) ester phthalic acid
$C_{24}H_{40}$	62155-50-4	14-094	(1-Cyclohexyldodecyl)benzene	1-Cyclohexyl-1-phenyldodecane
$C_{24}H_{46}CdO_4$	2605-44-9	74-010	Cadmium salt dodecanoic acid	Cadmium dodecanoate; Cadmium laurate
$C_{24}H_{46}HgO_4$	23186-25-6	74-011	Mercury (2+) salt dodecanoic acid	Mercury(II) dodecanoate; Mercury(II) laurate
$C_{24}H_{46}O_4Pb$	15773-55-4	74-012	Lead (2+) salt dodecanoic acid	Lead(II) dodecanoate; Lead(II) laurate
$C_{24}H_{50}$	646-31-1	11-064	Tetracosane	
$C_{24}H_{50}O_7$	3055-96-7	47-073 /S1	3,6,9,12,15,18-Hexaoxatriacontan-1-ol	Hexaoxyethylene glycol dodecyl ether
$C_{24}H_{51}N$	1116-76-3	31-065 /S1+S2	*N*,*N*-Dioctyl-1-octanamine	*N*,*N*,*N*-Trioctylamine
$C_{24}H_{52}ClNO_4$	4656-81-9	74-013	*N*,*N*,*N*-Trihexyl-1-hexanaminium perchlorate	Tetrahexylammonium perchlorate
$C_{24}H_{52}O_4Si$	78-13-7	71-051	Tetrakis(2-ethylbutyl) ester silicic acid	Tetrakis(2-ethylbutyl) orthosilicate; Tetrakis(2-ethylbutoxy)silane
$C_{25}H_{34}O_2S$	61519-00-4	63-008 /S1	*S*- (4-Pentylphenyl) ester 4-(heptyloxy)benzenecarbothioic acid	4-*n*-Pentylphenyl-4′-heptyloxythiobenzoate
$C_{25}H_{42}O_3$	15872-50-1	47-074 /S1	4-(Octadecyloxy)benzoic acid	*p*-*n*-Octadecyloxybenzoic acid
$C_{25}H_{44}$	29136-19-4	14-125 /S1	Nonadecylbenzene	
$C_{25}H_{46}$		12-122	4′-Heptyl-1,1′:3′,1″-tercyclohexane	4-Heptyl-*m*-tercyclohexyl
$C_{25}H_{46}O_6$	33599-07-4	45-111	2,3-Bis(acetyloxy)propyl ester octadecanoic acid	1,2-Diacetostearin
$C_{25}H_{48}O_4$	103-24-2	45-112	Bis(2-ethylhexyl) nonanedioate	Bis(2-ethylhexyl) azelate; Bis(2-ethylhexyl) ester nonanedioic acid
$C_{25}H_{50}$	22349-03-7	12-136 /S1	Nonadecylcyclohexane	
$C_{25}H_{52}$	629-99-2	11-065	Pentacosane	
$C_{25}H_{55}NO_9S$	872672-63-4	75-049 /S2	*N*-[2-[2-(2-Hydroxyethoxy)ethoxy]ethyl]-*N*-[(2-hydroxyethoxy)ethyl]-*N*-methyl -1-tridecanaminium methylsulfate	[ECOENG 500]
$C_{26}H_{18}$	1499-10-1	14-095 /B+S1	9,10-Diphenylanthracene	
$C_{26}H_{26}OSi_2$	807-28-3	71-052	1,3-Dimethyl-1,1,3,3-tetraphenyl-disiloxane	
$C_{26}H_{36}O_3Si_3$	1438-86-4	71-053	2,2-Dimethyl-4,4,6,6-tetraphenylcyclo-trisiloxane	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{26}H_{38}N_2O_3$	2635-26-9	62-122	Bis(4-heptyloxyphenyl)diazene-1-oxide	4,4′-Bis(heptyloxy) azoxybenzene
$C_{26}H_{41}N_3O_2$	218765-45-8	62-187 /S2	Tetradecanoic acid comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1)	
$C_{26}H_{50}O_4$	2432-87-3	45-113	Dioctyl decanedioate	Dioctyl ester decanedioic acid; Dioctyl sebacate
$C_{26}H_{50}O_4Pb$	50354-80-8	74-031 /S1	Lead (2+) salt tridecanoic acid	Lead(II) tridecanoate
$C_{26}H_{54}$	630-01-3	11-066	Hexacosane	
$C_{26}H_{54}O_9$	24233-81-6	47-075 /S1	3,6,9,12,15,18,21,24-Octaoxatetra-triacontan-1-ol	Octaoxyethylene glycol decyl ether
$C_{27}H_{46}O$	57-88-5	42-125 /S1	Cholesterol	5-Cholesten-3β-ol
$C_{27}H_{48}$	481-21-0	12-137 /S1	(5α)-Cholestane	17-(1,5-Dimethylhexyl)-10,13-dimethylhexahydro-1*H*-cyclopenta[*a*]phenanthrene
	6703-80-6	14-096	11-Phenylheneicosane	(1-Decylundecyl)benzene; 11-Phenylhenicosane
$C_{27}H_{50}$		12-123	4′-Nonyl-1,1′:3′,1″-tercyclohexane	4-Nonyl-*m*-tercyclohexyl
$C_{27}H_{50}O_6$	538-23-8	45-114	1,2,3-Propanetriyl ester octanoic acid	1,2,3-Propanetriyl trioctanoate; Trioctanoin
$C_{27}H_{54}$	6703-99-7	12-124	(1-Decylundecyl)cyclohexane	11-Cyclohexylheneicosane; 11-Cyclohexylhenicosane
$C_{27}H_{54}AsN_3S_6$	48233-55-2	73-050 /S1	Tris(dibutylcarbamodithioato-*S*,*S*′) arsenic	
$C_{27}H_{54}BiN_3S_6$	34410-99-6	73-051 /S1	Tris(dibutylcarbamodithioato-*S*,*S*′) bismuth	
$C_{27}H_{54}InN_3S_6$	23467-56-3	73-053 /S1	Tris(dibutylcarbamodithioato-*S*,*S*′) indium	
	85129-27-7	73-052 /S1	Tris[bis(2-methylpropyl)carbamodi-thiato-*S*,*S*′]indium	
$C_{27}H_{54}N_3PS_6$	69267-83-0	72-019 /S1	Tris(anhydrosulfide) with phosphorotrithious acid dibutylcarbamodithioic acid	
$C_{27}H_{54}N_3S_6Sb$	14907-93-8	73-054 /S1	Tris(dibutylcarbamodithioato-*S*,*S*′) antimony	
$C_{27}H_{56}$	593-49-7	11-067	Heptacosane	
$C_{28}H_{28}P$	7688-25-7	72-015	1,4-Butanediylbis(diphenylphosphine)	1,4-Bis(diphenylphosphino)butane; Tetramethylenebis (diphenylphosphine)
$C_{28}H_{32}O_4Si_4$	1693-47-6	71-054	2,2,4,4-Tetramethyl-6,6,8,8-tetraphenyl cyclotetrasiloxane	
	77-63-4	71-055	2,4,6,8-Tetramethyl-2,4,6,8-tetraphenyl cyclotetrasiloxane	
$C_{28}H_{42}N_2O_3$	25729-12-8	62-123	Bis(4-octyloxyphenyl)diazene-1-oxide	4,4′-Bis(octyloxy)azoxybenzene
$C_{28}H_{54}CdO_4$	10196-67-5	74-014	Cadmium salt tetradecanoic acid	Cadmium tetradecanoate; Cadmium myristate
$C_{28}H_{54}HgO_4$	36215-49-3	74-015	Mercury (2+) salt tetradecanoic acid	Mercury(II) tetradecanoate; Mercury(II) myristate
$C_{28}H_{54}O_2$	3687-46-5	45-152 /S1	Decyl ester (*Z*)-9-octadecenoic acid	Decyl oleate
$C_{28}H_{54}O_4Pb$	32112-52-0	74-016	Lead (2+) salt tetradecanoic acid	Lead(II) tetradecanoate; Lead(II) myristate
$C_{28}H_{58}$	630-02-4	11-068	Octacosane	
$C_{29}H_{42}O_4$	68162-09-4	47-050	4-(Hexyloxy)phenyl ester 4-(decyloxy)benzoic acid	4-Hexyloxyphenyl-4′-*n*-decyloxybenzoate
$C_{29}H_{44}O_6Si_2$	349149-95-7	71-070 /S2	4-Methoxy-4-[[1-oxo-11-(1,1,3,3-tetra methyldisiloxanyl)undecyl]oxy]phenyl ester benzoic acid	
	179108-75-9	71-071 /S2	4-Methoxyphenyl ester 4-[[1-oxo-11-(1,1,3,3-tetramethyldisilo xanyl)undecyl]oxy]benzoic acid	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{30}H_{32}P_2$	19845-69-3	72-020 /S1	1,6-Hexanediyl[diphenylphosphine]	1,6-Bis(diphenylphosphino) hexane
$C_{30}H_{46}N_2O_3$	25729-13-9	62-124	Bis(4-nonyloxyphenyl)diazene-1-oxide	4,4′-Bis(nonyloxy)azoxybenzene
$C_{30}H_{58}O_4$	2432-89-5	45-115	Didecyl decanedioate	Didecyl ester decanedioic acid; Didecyl sebacate
$C_{30}H_{61}Br$	4209-22-7	23-040	1-Bromotriacontane	*n*-Triacontyl bromide
$C_{30}H_{62}$	111-01-3	11-069	2,6,10,15,19,23-Hexamethyltetracosane	Squalane
	638-68-6	11-070	Triacontane	
$C_{31}H_{32}O_2P_2$	32305-98-9	72-021 /S1	[[(4*R*,5*R*)-2,2-Dimethyl-1,3-dioxolane-4,5-diyl]bis(methylene)]bis(diphenylphosphine)	(-)-2,3-*O*-Isopropylidene-2,3-dihydroxy-1,4-bis (diphenylphosphino)butane
$C_{31}H_{52}O_3$	7695-91-2	47-051	3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2*H*-1-benzopyran-6-ol acetate	α-Tocopherol acetate
$C_{31}H_{62}O$	502-73-8	43-070 /S1	16-Hentriacontanone	Dipentadecyl ketone
$C_{31}H_{64}$	55320-06-4	11-071	11-Decylheneicosane	11-Decylhenicosane
	630-04-6	11-072	Hentriacontane	Unatriacontane
$C_{32}H_{50}N_2O_3$	2312-12-1	62-125	Bis(4-decyloxyphenyl)diazene-1-oxide	4,4′-Bis(decyloxy) azoxybenzene
$C_{32}H_{54}O_4$	40989-56-8	45-153 /S1	Bis(2,4-diethyloctyl) ester 1,2-benzenedicarboxylic acid	Diisododecyl phthalate
$C_{32}H_{62}CdO_4$	6427-86-7	74-017	Cadmium salt hexadecanoic acid	Cadmium hexadecanoate; Cadmium palmitate
$C_{32}H_{62}HgO_4$	16888-60-1	74-018	Mercury (2+) salt hexadecanoic acid	Mercury(II) hexadecanoate; Mercury(II) palmitate
$C_{32}H_{62}O_4Pb$	15773-56-5	74-019	Lead (2+) salt hexadecanoic acid	Lead(II) hexadecanoate; Lead(II) palmitate
$C_{32}H_{66}$	544-85-4	11-073	Dotriacontane	
$C_{33}H_{62}O_6$	621-71-6	45-116	1,2,3-Propanetriyl ester decanoic acid	1,2,3-Propanetriyl tridecanoate; Tridecanoin
$C_{33}H_{68}$	630-05-7	11-074	Tritriacontane	
$C_{34}H_{54}N_2O_3$	2312-13-2	62-126	Bis[4-(undecyloxy)phenyl]diazene-1-oxide	4,4′-Bis(undecyloxy) azoxybenzene
$C_{34}H_{66}O_4$	2432-88-4	45-117	Didodecyl decanedioate	Didodecyl ester decanedioic acid; Didodecyl sebacate
$C_{34}H_{70}$	14167-59-0	11-075	Tetratriacontane	
$C_{35}H_{72}$	630-07-9	11-076	Pentatriacontane	
$C_{36}H_{24}$	7059-70-3	14-097	1,1′,1″-(1,3,5-Benzenetriyl) tris(naphthalene)	1,3,5-Tri-α-naphthylbenzene
$C_{36}H_{46}O_5$	103376-72-3	47-086 /S2	4′-(Octyloxy)-4-[[(1-methylheptyl)oxy] carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid	
$C_{36}H_{48}N_2O_2$	29273-90-3	62-174 /S1	(*E*,*E*)−*N*,*N*′-Bis[[4-(octyloxy)phenyl] methylene]-1,4-benzenediamine	*N*,*N*′-Bis(4-*n*-octyloxybenzal)-1,4-phenylenediamine
$C_{36}H_{54}O_{12}$	65201-68-5	45-186 /S2	1,2,3,4,5,6-Benzenehexayl ester pentanoic acid	Benzene hexa-*n*-pentanoate
$C_{36}H_{58}N_2O_3$	2312-14-3	62-127	Bis[4-(dodecyloxy)phenyl]diazene-1-oxide	4,4′-Bis(dodecyloxy) azoxybenzene
$C_{36}H_{68}O_2$	3687-45-4	45-154 /S1	(*Z*)-9-Octadecenyl ester (*Z*)-9-octadecenoic acid	Oleyl oleate
$C_{36}H_{70}CdO_4$	2223-93-0	74-020	Cadmium salt octadecanoic acid	Cadmium octadecanoate; Cadmium stearate
$C_{36}H_{70}HgO_4$	645-99-8	74-021	Mercury (2+) salt octadecanoic acid	Mercury(II) octadecanoate; Mercury(II) stearate
$C_{36}H_{70}O_4Pb$	1072-35-1	74-022	Lead (2+) salt octadecanoic acid	Lead(II) octadecanoate; Lead(II) stearate
$C_{36}H_{73}NO_7S$	663955-05-3	75-050 /S2	*N*,*N*,*N*-Tributyl-1-butanaminium 1,4-bis(2-ethylhexyl)sulfobutanedioate	[N4444][doc]
$C_{36}H_{74}$	630-06-8	11-077 /B+S1	Hexatriacontane	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
$C_{37}H_{46}O_6$	135861-12-0	47-087 /S2	4′-[(1-Oxononyl)oxy]-4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid	MHPOCBC
$C_{37}H_{54}Si$	4033-52-7	71-056	Tribenzylhexadecylsilane	
$C_{38}H_{70}O_8$	55205-81-7	45-118	1,6-Hexanediyldihexyl ester decanedioic acid	Dihexyl hexamethylenesebacate
$C_{38}H_{74}O_4$	26719-47-1	45-119	Ditetradecyl decanedioate	Ditetradecyl ester decanedioic acid; Ditetradecyl sebacate
$C_{39}H_{74}O_6$	538-24-9	45-120 /B+S1+S2	1,2,3-Propanetriyl ester dodecanoic acid	1,2,3-Propanetriyl tridodecanoate; Trilaurin
$C_{39}H_{78}O$	22986-70-5	43-071 /S1	20-Nonatriacontanone	Dinonadecyl ketone
$C_{40}H_{82}$	4181-95-7	11-078	Tetracontane	
$C_{41}H_{72}O_2$	1989-52-2	45-121	Cholest-5-en-3-ol (3β) tetradecanoate	Cholesterol myristate
$C_{42}H_{66}O_{12}$	65201-69-6	45-122	1,2,3,4,5,6-Benzenehexayl ester hexanoic acid	Benzene hexa-*n*-hexanoate
$C_{42}H_{82}O_4$	26719-48-2	45-123	Dihexadecyl decanedioate	Dihexadecyl ester decanedioic acid; Dihexadecyl sebacate
$C_{42}H_{86}$	7098-20-6	11-079	Dotetracontane	
$C_{43}H_{88}$	7098-21-7	11-080	Tritetracontane	
$C_{44}H_{90}$	7098-22-8	11-081	Tetratetracontane	
$C_{45}H_{86}O_6$	555-45-3	45-124 /B+S1+S2	1,2,3-Propanetriyl ester tetradecanoic acid	1,2,3-Propanetriyl tritetradecanoate; Trimyristin
$C_{46}H_{90}O_4$	3072-03-5	45-125	Dioctadecyl decanedioate	Dioctadecyl ester decanedioic acid; Dioctadecyl sebacate
$C_{47}H_{90}O_6$	60138-13-8	45-155 /S1+S2	2,3-Bis[(1-oxotetradecyl)oxy]propyl ester hexadecanoic acid	1,2-Dimyristoyl-3-palmitoyl triglyceride
$C_{48}H_{40}P_2$	153305-67-0	72-022 /S1	[1,1′-Binaphthalene]-2,2′-diylbis[bis(4-methylphenyl)phosphine]	2,2′-Bis(di-*p*-toluenephosphino)-1,1′-binaphthyl
$C_{48}H_{78}O_{12}$	65201-70-9	45-126	1,2,3,4,5,6-Benzenehexayl ester heptanoic acid	Benzene hexa-*n*-heptanoate
$C_{48}H_{98}$	7098-26-2	11-082	Octatetracontane	
$C_{49}H_{92}O_6$	74160-01-3	45-156 /S1	2,3-Bis[(1-oxotetradecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid	1,2-Dimyristoyl-3-oleoyl triglyceride
$C_{50}H_{102}$	6596-40-3	11-083	Pentacontane	
$C_{51}H_{98}O_6$	555-44-2	45-127 /B+S1+S2	1,2,3-Propanetriyl ester hexadecanoic acid	1,2,3-Propanetriyl trihexadecanoate; Tripalmitin
$C_{53}H_{100}O_6$	1867-91-0	45-157 /S1	2,3-Bis[(1-oxohexadecyl)oxy]propyl ester (*Z*)-9-octadecenoic acid	1,2-Dipalmitoyl-3-oleoyl triglyceride
	2190-25-2	45-187 /S2	2-[(1-Oxohexadecyl)oxy]-1-[[(1-oxohexadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid	1,3-Dipalmitoyl-2-olein; POP
$C_{54}H_{84}O_6$	70351-86-9	41-057 /S2	2,3,6,7,10,11-Hexahexyloxy-triphenylene	
$C_{54}H_{90}O_{12}$	65201-71-0	45-128	1,2,3,4,5,6-Benzenehexayl ester octanoic acid	Benzene hexa-*n*-octanoate
$C_{54}H_{98}O_{12}$	55205-82-8	45-129	10,19,28,37-Tetraoxodihexyl ester 11,18,29,36-tetraoxahexatetra-cosanedioic acid	Dihexyl bis(hexamethylenesebacate)
$C_{55}H_{102}O_6$	2190-30-9	45-158 /S1+S2	1-[[(1-Oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (*Z*)-9-octadecenoic acid	1,2-Dioleoyl-3-palmitoyl triglyceride; 3-Palmito-1,2-diolein
$C_{55}H_{104}O_6$	2190-27-4	45-188 /S2	1-[[(1-Oxohexadecyl)oxy]methyl]-2-[(1-oxooctadecyl)oxy]ethyl ester (9*Z*)-9-octadecenoic acid	1-Palmito-3-stearo-2-olein; 1-Palmito-2-oleostearin; POS
$C_{57}H_{92}O_6$	14465-68-0	45-159 /S1	(all-*Z*)-1,2,3-Propanetriyl ester 9,12,15-octadecatrienoic acid	Trilinolein
$C_{57}H_{104}O_6$	537-39-3	45-189 /S2	1,2,3-Propanetriyl ester (9*E*,9′*E*,9″*E*)-9-octadecenoic acid	Trielaidin

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
	122-32-7	45-190 /S2	1,2,3-Propanetriyl ester (9*Z*)-9-octadecenoic acid	Triolein; Glycerin trioleate
$C_{57}H_{108}O_6$	2846-04-0	45-191 /S2	2-[(1-Oxooctadecyl)oxy]-1-[[(1-oxo octadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid	1,3-Distearoyl-2-olein; SOS
$C_{57}H_{110}O_6$	555-43-1	45-130 /B+S1+S2	1,2,3-Propanetriyl ester octadecanoic acid	1,2,3-Propanetriyl trioctadecanoate; Tristearin
$C_{60}H_{102}O_{12}$	65201-72-1	45-192 /S2	1,2,3,4,5,6-Benzenehexayl ester nonanoic acid	
$C_{66}H_{96}O_{12}$	70351-94-9	45-160 /S1	2,3,6,7,10,11-Triphenylenehexayl ester octanoic acid	2,3,6,7,10,11-Hexa-*n*-octanoyloxy triphenylene
$C_{66}H_{114}O_{12}$	65201-73-2	45-193 /S2	1,2,3,4,5,6-Benzenehexayl ester decanoic acid	
ClD	7698-05-7	02-030	Hydrochlorid acid-*d*	Deuterium chloride
$ClFO_3$	7616-94-6	02-031 /B+S1	Perchloryl fluoride ($(ClO_3)F$)	
ClF_3	13637-63-3	02-032	Chlorine fluoride (ClF_3)	Chlorine trifluoride
ClH	7647-01-0	02-033	Hydrochlorid acid	Hydrogen chloride
$ClHO_4$	7601-90-3	02-034	Perchloric acid	
ClI	7790-99-0	02-035	Iodine chloride	Iodine monochloride
$ClNaO_3$	7775-09-9	02-036	Sodium salt chloric acid	Sodium chlorate
Cl_2	7782-50-5	01-004	Chlorine	
Cl_2OS	7719-09-7	02-037	Thionyl chloride	
Cl_2O_2S	7791-25-5	02-038	Sulfuryl chloride	
$Cl_2O_5S_2$	7791-27-7	02-039	Disulfuryl chloride	Pyrosulfuryl chloride
Cl_2S_2	10025-67-9	02-040	Sulfur chloride (S_2Cl_2)	Sulfur monochloride
Cl_2Sn	7772-99-8	02-041	Tin chloride ($SnCl_2$)	
Cl_3HSi	10025-78-2	02-042	Trichlorosilane	
Cl_3OP	10025-87-3	02-043	Phosphoryl chloride	
Cl_3P	7719-12-2	02-044	Phosphorous trichloride	Phosphorus chloride (PCl_3)
Cl_4Ge	10038-98-9	02-045	Tetrachlorogermane	Germanium tetrachloride
Cl_4Si	10026-04-7	02-046	Tetrachlorosilane	Silicon chloride
Cl_4Sn	7646-78-8	02-047	Tetrachlorostannane	Tin(IV) chloride; Tin tetrachloride
Cl_4Te	10026-07-0	02-048	Tellurium chloride ($TeCl_4$)	Tellurium tetrachloride
Cl_4Ti	7550-45-0	02-049	Titanium chloride ($TiCl_4$)	Titanium tetrachloride; Titanic chloride
$Cl_6N_3P_3$	940-71-6	02-104 /S1	2,2,4,4,6,6-Hexachloro-2,2,4,4,6,6-hexa hydro-1,3,5,2,4,6-triazatriphosphorine	Hexachlorocyclotriphosphazene
$Cl_8N_4P_4$	2950-45-0	02-105 /S1	2,2,4,4,6,6,8,8-Octachloro-2,2,4,4,6,6,8, 8-octahydro-1,3,5,7,2,4,6,8-tetrazatetra phosphorine	Octachlorocyclotetra-phosphazene
Cs	7440-46-2	01-005	Cesium	
CsF_2H	12280-52-3	02-050	Cesium fluoride ($Cs(HF_2)$)	Cesium hydrogen difluoride
DH	13983-20-5	02-051	Hydrogen deuteride	
DI	14104-45-1	02-052	Hydroiodic acid-*d*	Deuterium iodide
D_2	7782-39-0	01-006 /B+S1	Deuterium (D_2)	
		01-007	*ortho*-Deuterium (D_2)	
D_2O	7789-20-0	02-053 /B+S2	Water-d_2	Heavy water; Deuterium oxide
D_2O_2	6909-54-2	02-054	Hydrogen-d_2 peroxide	Deuterium peroxide
D_2S	13536-94-2	02-055	Hydrogen sulfide-d_2	Deuterium sulphide
D_2Se	13536-95-3	02-056	Hydrogen selenide-d_2	Deuterium selenide
D_3N	13550-49-7	02-057	Ammonia-d_3	Deuterium ammonia; Trideuterated ammonia
FH	7664-39-3	02-058	Hydrofluoric acid	Hydrogen fluoride
F_2	7782-41-4	01-008	Fluorine	
F_2HRb	12280-64-7	02-059	Rubidium fluoride ($Rb(HF_2)$)	Rubidium hydrogen difluoride
F_2H_5N	1341-49-7	02-060	Ammonium fluoride ($(NH_4)(HF_2)$)	Ammonium hydrogen difluoride
F_2O	7783-41-7	02-061	Oxygen fluoride	

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
F_2OS	7783-42-8	02-062	Thionyl fluoride	
F_2O_2S	2699-79-8	02-063 /B+S1	Sulfuryl fluoride	
F_3N	7783-54-2	02-064	Nitrogen fluoride (NF_3)	Nitrogen trifluoride
F_3OP	13478-20-1	02-065	Phosphoryl fluoride	
F_3P	7783-55-3	02-066	Phosphorous trifluoride	Phosphorus trifluoride; Phosphorous fluoride (PF_3)
F_4Si	7783-61-1	02-106 /S1	Tetrafluorosilane	Silicon tetrafluoride
F_5I	7783-66-6	02-067	Iodine fluoride (IF_5)	Iodine pentafluoride
F_5Nb	7783-68-8	02-068	Niobium fluoride (NbF_5)	Niobium pentafluoride
F_6Mo	7783-77-9	02-069	Molybdenum fluoride (MoF_6)	Molybdenum hexafluoride
F_6S	2551-62-4	02-070 /B+S1	Sulfur fluoride (SF_6)	Sulfur hexafluoride
F_6Se	7783-79-1	02-107 /S1	Selenium fluoride (SeF_6)	Hexafluoroselenium
F_6U	7783-81-5	02-071	Uranium(VI) fluoride	Uranium hexafluoride
F_6W	69175-55-9	02-108 /S1	Tungsten fluoride (WF_6)	Hexafluorotungsten
Ga	7440-55-3	01-009 /B+S2	Gallium	
GeH_4	7782-65-2	02-072 /B+S1	Germane	
HI	10034-85-2	02-073	Hydroiodic acid	Hydrogen iodide
HNO_3	7697-37-2	02-074	Nitric acid	
H_2	1333-74-0	01-010	Hydrogen	
		01-011	*para*-Hydrogen	
H_2O	7732-18-5	02-075	Water	
H_2O_2	7722-84-1	02-076	Hydrogen peroxide	
H_2O_4S	7664-93-9	02-077	Sulfuric acid	
$H_2O_7S_2$	7783-05-3	02-078	Disulfuric acid	Pyrosulfuric acid
$H_2{}^{18}O$	14314-42-2	02-109 /S1	Water-^{18}O	Heavy Oxygen Water
H_2S	7783-06-4	02-079	Hydrogen sulfide	
H_2S_2	13465-07-1	02-080	Hydrogen sulfide (H_2S_2)	Dihydrogen disulfide
H_2S_3	13845-23-3	02-081	Hydrogen sulfide (H_2S_3)	Dihydrogen trisulfide
H_2S_4	13845-25-5	02-082	Hydrogen sulfide (H_2S_4)	Dihydrogen tetrasulfide
H_2S_5	13845-24-4	02-083	Hydrogen sulfide (H_2S_5)	Dihydrogen pentasulfide
H_2S_6	13845-51-7	02-084	Hydrogen sulfide (H_2S_6)	Dihydrogen hexasulfide
H_2Se	7783-07-5	02-085	Hydrogen selenide	
H_3N	7664-41-7	02-086 /B+S1	Ammonia	
H_3O_4P	7664-38-2	02-087	Phosphoric acid	
H_3P	7803-51-2	02-088	Phosphine	
H_4N_2	302-01-2	02-089	Hydrazine	
H_4Si	7803-62-5	02-090	Silane	
H_5NO	1336-21-6	02-091	Ammonium hydroxide	
$H_5N_3O_3$	13464-97-6	02-092	Hydrazine mononitrate	Hydrazine nitrate
H_8N_2O	12161-77-2	02-093	Ammonium oxide	
He	14762-55-1	01-013	Helium (isotope of mass 3)	
He	7440-59-7	01-012	Helium	
Hg	7439-97-6	01-014	Mercury	
HgI_2	7774-29-0	02-094	Mercury iodide (HgI_2)	
I_2	7553-56-2	01-015	Iodine	
I_4Sn	7790-47-8	02-095	Tetraiodostannane	Tin iodide; Stannic iodide
In	7440-74-6	01-016	Indium	
K	7440-09-7	01-017	Potassium	Kalium
Kr	7439-90-9	01-018	Krypton	
Li	7439-93-2	01-019	Lithium	
$LiNO_3$	7790-69-4	02-096	Lithium salt nitric acid	Lithium nitrate
NO	10102-43-9	02-097	Nitrogen oxide (NO)	Nitrogen monoxide; Nitric oxide
NO_2	10102-44-0	02-098	Nitrogen oxide (NO_2)	Nitrogen dioxide
N_2	7727-37-9	01-020	Nitrogen	
N_2O	10024-97-2	02-099 /B+S1	Nitrogen oxide (N_2O)	Dinitrogen monoxide; Nitrous oxide

TABLE 5. Formula index of compounds—Continued

Formula	CAS Registry Number	Group-Member Number	Name	Synonyms, Common Names, or Commercial Names
N_2O_4	10544-72-6	02-100	Nitrogen oxide (N_2O_4)	Dinitrogen tetroxide; Nitrogen peroxide; Nitrogen tetroxide
Na	7440-23-5	01-021	Sodium	Natrium
Ne	7440-01-9	01-022	Neon	
O_2	7782-44-7	01-023	Oxygen	
O_2S	7446-09-5	02-101	Sulfur dioxide	
O_3	10028-15-6	01-024	Ozone	
O_3S	7446-11-9	02-102	Sulfur trioxide	
O_6P_4	12440-00-5	02-103	Phosphorus oxide (P_4O_6)	
P_4	12185-10-3	01-025	Phosphorus mol.(P_4)	
Rb	7440-17-7	01-026	Rubidium	
S	7704-34-9	01-027	Sulfur	
Se	7782-49-2	01-028	Selenium	
Sn	7440-31-5	01-029	Tin	Stannane
Xe	7440-63-3	01-030	Xenon	

6. Heat capacity datasheets

6.1. Main group 0: inorganic compounds

6.1.1. Sub group 01: elements

6.1.1.1. Gallium (1-009)

Name:	Gallium
Formula:	Ga
CAS-RN:	7440-55-3
Group No:	1-009

Experimental heat capacities (1.9.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Method
1933ROT/MEY2	N	298.1–313.1	2		n/a	n/a	n/a	*p*	DSIO	1933ROT/MEY2
1934ROT/MEY	N	298.1–373.1	2	S	n/a	n/a	n/a	avg	DSIO	1933ROT/MEY2
1952ADA/JOH		306.9–322.8	4		n/a	99.98	melpt	*p*	BSAO	1952ADA/JOH
1969BOI/BRO		302.9–307.6	7		0.40	99.9999	anal	*p*	BDCT	1965STE/CAL
1983TAK/KAD		298.3–613.4	87		1.00	99.9999	anal	*p*	BDHO	1979TAK/YOK
1984AMI/MIN		304.4–319.2	27		n/a	99.9999	anal	*p*	BSAO	1979AMI/LEB

Reference	Notes
1933ROT/MEY2	constant value calculated from temperature dependence of enthalpy by the authors; correct data in 1934ROT/MEY
1934ROT/MEY	corrected datum in 1933ROT/MEY2; a constant value calculated from temperature dependence of enthalpy by the authors

6.1.2. Sub group 02: inorganic compounds

6.1.2.1. Silver(1+) salt nitric acid (2-001)

Name:	Silver(1+) salt nitric acid
Formula:	$AgNO_3$
CAS-RN:	7761-88-8
Group No:	2-001

Experimental heat capacities (2.1.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1907GUI2	N	502.1	1	n/a	n/a	n/a	avg	DSIO	1907GUI2
1909GOO/KAL	N	491.1–541.2	2	n/a	n/a	n/a	avg	DSIO	1909GOO/KAL
1963JAN/KEL		528.5	1	1.00	n/a	n/a	*p*	DSIO	1958GOO/SOL
1998ZAM/ROG		514.0–517.0	4	0.50	99.995	anal	*p*	BDHT	1992HWA/DES

Reference	Notes
1907GUI2	average value in the temperature range 481–523 K
1909GOO/KAL	constant value calculated from temperature dependence of enthalpy by the authors

Correlated heat capacities (2.1.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1909GOO/KAL	491.1–541.2	2	1.00	#	0.383	6.38−2	0.38	6.38−2	2
1998ZAM/ROG	514.0–517.0	4	0.50		0.095	7.91−3	0.05	−7.91−3	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1907GUI2	(6.20−1, 3.88, −6.20−1, −1)	1963JAN/KEL	(2.52, 17.89, −2.52, −1)	

Parameters of regression polynomial (2.1.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	8	6	0.257	4.10−2	0.25	1.60−2	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
491.1–541.2	1.660 55+1				IV

Deviation plot for Silver(1+) salt nitric acid (2–001) is given in Fig. 1.

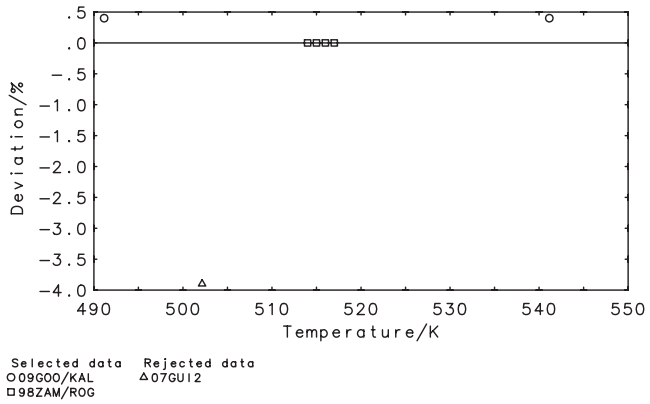

FIG. 1. Deviation plot for silver(1+) salt nitric acid (2-001).

6.1.2.2. Water-d_2 (2-053)

Name:	Water-d_2
Formula:	D_2O
CAS-RN:	7789-20-0
Group No:	2-053

Experimental heat capacities (2.53.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1935BAR/CLU	N	284.1	1		1.00	99.7	anal	avg	DSTO	1935BAR/CLU
1935BRO/BAR1	N	287.6	1		1.00	98.	anal	avg	DSAO	1930BAR/MAA
1935BRO/BAR2	N	288.1–318.6	3		1.00	98.	Anal	avg	DSAO	1930BAR/MAA
1935JAC	N	276.9	1		n/a	97.7	Anal	sat	BSIO	1935JAC
1936LON/KEM		279.4–295.2	4		0.20	99.997	melpt	*p*	BSIO	1936GIA/STO
1940COC/FER	N	285.1–325.8	31		n/a	99.2	Anal	sat	BDHO	1940COC/FER
1951EUC/EIG	N	293.0–398.0	12	S	n/a	96.	estim	sat	BSAO	1951EUC/EIG
1959BAK	N	304.0–473.1	37		n/a	99.77	Anal	sat	BSIO	1959BAK
1970KRE		298.1	1		n/a	99.7	Anal	*p*	BSAO	1963BEN
2006SMI/BYK		278.5–346.1	24		0.20	99.997	melpt	*p*	BSAO	1997VAR/DRU1

Reference	Notes
1935BAR/CLU	average value in the temperature range 277–291 K
1935BRO/BAR1	average value in the temperature range 277–298 K
1935BRO/BAR2	average values in the temperature ranges 277–299, 299–318, and 299–338 K
1935JAC	value extrapolated to 100% D_2O
1940COC/FER	preliminary data published in 1936FER/COC
1951EUC/EIG	purity was estimated from density by the authors
1959BAK	data in the temperature range 373–473 K measured in an isoperibol calorimeter (but not described)

Correlated heat capacities (2.53.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1940COC/FER	285.1–325.8	31	0.50	#	0.667	3.37−2	0.33	2.29−2	21
1951EUC/EIG	293.0–398.0	11	1.00	#	0.160	1.61−2	0.16	8.48−3	1
1959BAK	304.0–473.1	37	0.70	#	1.193	8.47−2	0.83	3.45−2	12
1970KRE	298.1	1	1.00	#	0.165	1.67−2	0.17	1.67−2	1
2006SMI/BYK	278.5–346.1	24	0.50	#	1.404	7.01−2	0.70	−5.55−2	−16

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1935BAR/CLU	(1.02, 11.20, −1.02, −1)	1935BRO/BAR1	(2.00−1, 1.93, 2.00−1, 1)
1935BRO/BAR2	(8.52−2, 0.84, 7.63−2, 3)	1936LON/KEM	(1.19−1, 1.19, −1.08−1, −4)

Parameters of regression polynomial (2.53.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	115	104	1.068	6.49−2	0.64	7.36−3	19
sat	115	104	1.067	6.49−2	0.64	7.35−3	19

T/K	A_1	A_2	A_3	A_4	Uncert.
278.5–473.1	8.282 94	2.833 06	−1.160 21	1.398 20−1	IV
278.5–473.1	8.797 44	2.349 84	−1.009 20	1.241 13−1	IV

Deviation plot for Water-d_2 (2–053) is given in Fig. 2.

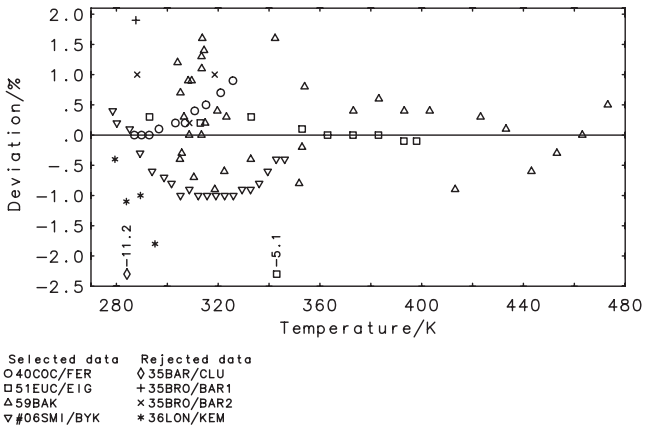

FIG. 2. Deviation plot for water-d_2 (2-053).

6.2. Main group 1: compounds of carbon and hydrogen

6.2.1. Sub group 11: saturated aliphatic hydrocarbons

6.2.1.1. Pentane (11-010)

Name:	Pentane
Formula:	C_5H_{12}
CAS-RN:	109-66-0
Group No:	11-010

Experimental heat capacities (11.10.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930PAR/HUF1		149.9–290.0	14		1.00	n/a	n/a	*p*	BSIO	1925PAR
1940MES/KEN		151.3–286.4	19		n/a	99.961	melpt	*p*	BSAO	1939AST/EID1
1967MES/GUT		148.6–302.9	25		0.10	99.86	melpt	sat	BSAO	1947HUF
1971AMI/ALI	N	313.1–468.1	19	S	2.00	n/a	n/a	*p*	n/a	n/a
1975GRI/RAS	N	299.9–383.6	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1985CZA		299.0	1		n/a	n/a	n/a	*p*	BSIO	1979CZA
1988MEL/VER		153.1–433.1	10		2.50	n/a	n/a	sat	n/a	n/a
2005HUA/SIM		213.0–298.0	eqn		n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1971AMI/ALI	calculated from C_v measured at the saturation line
1975GRI/RAS	all values (except the first one) at pressures above the vapour pressure

6.2.1.2. Hexane (11-013)

Name:	Hexane
Formula:	C_6H_{14}
CAS-RN:	110-54-3
Group No:	11-013

Experimental heat capacities (11.13.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930PAR/HUF2		183.5–295.1	8		n/a	n/a	n/a	*p*	BSIO	1925PAR
1931HUF/PAR		188.8–293.5	5		1.00	n/a	n/a	*p*	BSIO	1925PAR
1937STU		180.0–320.0	15	S	n/a	n/a	n/a	*p*	BDHO	1937STU

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1939PHI		300.6	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1946DOU/HUF2	N	180.4–301.0	24		0.10	99.992	melpt	*p*	BSAO	1943RUE/HUF
1951CON/SAG		299.8–366.5	13	S	0.70	n/a	n/a	*p*	BSAO	1939SAG/EVA
1969WIL/ROT		293.1	1		0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1971AMI/ALI	N	343.1–506.1	19	S	2.00	n/a	n/a	*p*	n/a	n/a
1971REC/SAD		303.1	1		0.30	n/a	n/a	*p*	BSIO	1970REC
1974DIA/REN		298.2–324.7	14		0.30	n/a	n/a	*p*	BSAO	1974DIA/REN
1975GRI/RAS	N	304.5–463.1	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1976KAR/GRO		298.2	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1980KAL/JED		180.6–301.4	33		0.20	99.95	chrom	*p*	BSAO	1980KAL/JED
1981GRO/ING		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1982WIL/ING		298.1	1		n/a	99.5	estim	*p*	FSIT	1971PIC/LED
1982ZAR		298.0–323.0	2		0.60	n/a	n/a	*p*	BDCT	1982ZAR
1984BEN/DAR		298.1	1		n/a	99.98	melpt	*p*	FSIT	1971PIC/LED
1984BRA/PIN		298.1	1		n/a	99.0	melpt	*p*	FSIT	1971PIC/LED
1985COS/PAT1		298.2	1		n/a	99	anal	*p*	FSIT	1971PIC/LED
1985COS/PAT8		298.1–313.1	2		n/a	99	estim	*p*	FSIT	1971PIC/LED
1985CZA		299.9	1		n/a	n/a	n/a	*p*	BSIO	1979CZA
1986BEN/DAR1		298.1	1		n/a	99.88	Anal	*p*	FSIT	1971PIC/LED
1986NAZ/BAS2		308.4–333.1	2		2.00	99.8	estim	*p*	BDHO	1986NAZ/BAS1
1988MEL/VER		183.1–473.1	11		2.50	n/a	n/a	sat	n/a	n/a
1988SAI/TAN		298.1	1		n/a	99.95	Anal	*p*	FSIT	1971PIC/LED
1989OHN/FUJ		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA
1989VOG/SCH		333.1	1		n/a	n/a	n/a	*p*	BDHT	1969PER/COM
1991OGA/MIT		298.1	1		n/a	n/a	n/a	*p*	FSIO	1985OGA
1991PES/NIK	N	298.1	1		n/a	n/a	n/a	*p*	BSAO	1983KUK/KOR
1991TRE/COS		298.1	1		n/a	99.	Anal	*p*	FSIT	1971PIC/LED
1993CON/GIR1		298.0–333.0	eqn		5.00	n/a	n/a	sat	BDHT	1993CON/GIR1
2000BES/SAI2	N	313.1–333.1	3		1.00	n/a	n/a	*p*	BDCT	2000BES/SAI2
2001CER/TOV2		288.1–333.1	5		n/a	99.5	chrom	*p*	BDHT	1969PER/COM
2002PAR/ZOU		278.1–348.1	15		n/a	99.5	chrom	sat	BDCT	1983ROU/ROU
2005HUA/SIM		213.0–304.0	eqn		n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1946DOU/HUF2	smoothed data in 1967MES/GUT
1971AMI/ALI	calculated from C_v measured at the saturation line
1975GRI/RAS	all values (except the first one) at pressures above the vapor pressure
1991PES/NIK	water content below 0.05%
2000BES/SAI2	data measured at elevated pressure up to 100 MPa

Correlated heat capacities (11.13.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1931HUF/PAR	188.8–293.5	5	1.00		0.191	4.34−2	0.19	−2.70−2	−3
1946DOU/HUF2	180.4–301.0	24	0.10		0.729	1.55−2	0.07	2.27−4	1
1951CON/SAG	299.8–366.5	13	0.70		0.742	1.36−1	0.52	1.17−1	11
1969WIL/ROT	293.1	1	0.40		0.864	8.03−2	0.35	−8.03−2	−1
1975GRI/RAS	304.5–463.1	9	1.00		0.431	1.18−1	0.43	3.34−2	1
1976KAR/GRO	298.2	1	0.50	#	0.609	7.19−2	0.30	7.19−2	1
1980KAL/JED	180.6–301.4	33	0.50	#	0.542	5.74−2	0.27	1.13−2	4
1981GRO/ING	298.1	1	0.50	#	0.158	1.86−2	0.08	1.86−2	1

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1982WIL/ING	298.1	1	0.50	#	0.189	2.23−2	0.09	−2.23−2	−1
1982ZAR	298.0–323.0	2	0.60		0.044	6.22−3	0.03	4.70−3	1
1984BEN/DAR	298.1	1	0.50	#	0.291	3.43−2	0.15	3.43−2	1
1984BRA/PIN	298.1	1	0.50	#	0.189	2.23−2	0.09	−2.23−2	−1
1986BEN/DAR1	298.1	1	0.50	#	0.332	3.91−2	0.17	3.91−2	1
1988MEL/VER	183.1–413.1	10	2.50		0.123	7.47−2	0.31	5.53−3	0
1988SAI/TAN	298.1	1	0.50	#	0.128	1.50−2	0.06	1.50−2	1
1989OHN/FUJ	298.1	1	0.30	#	0.504	3.55−2	0.15	−3.55−2	−1
1991PES/NIK	298.1	1	0.30	#	0.655	4.63−2	0.20	4.63−2	1
2000BES/SAI2	313.1–333.1	3	1.00		0.141	3.51−2	0.14	3.40−2	3
2001CER/TOV2	288.1–333.1	5	0.40	#	0.312	3.09−2	0.13	−9.60−3	0
2002PAR/ZOU	278.1–348.1	15	0.50	#	0.864	1.05−1	0.43	−8.47−2	−15

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1930PAR/HUF2	(2.26−1, 1.02, −2.07−1, −8)	1937STU	(1.25, 5.22, 6.42−1, 4)
1939PHI	(1.24, 5.55, −1.24, −1)	1971AMI/ALI	(4.31−1, 1.49, −2.18−1, −4)
1971REC/SAD	(2.85−1, 1.22, −2.85−1, −1)	1974DIA/REN	(6.57−1, 2.60, 5.95−1, 14)
1985COS/PAT1	(2.56−1, 1.08, 2.56−1, 1)	1985COS/PAT8	(3.02−1, 1.23, 1.78−1, 0)
1985CZA	(1.62−1, 0.69, −1.62−1, −1)	1986NAZ/BAS2	(5.55−1, 2.20, 5.49−1, 2)
1989VOG/SCH	(8.70−1, 3.35, 8.70−1, 1)	1991OGA/MIT	(1.64−1, 0.69, 1.64−1, 1)
1991TRE/COS	(2.58−1, 1.09, 2.58−1, 1)	1993CON/GIR1	(1.42, 5.49, 1.41, 3)
2005HUA/SIM	(3.10−1, 1.35, 1.60−1, 4)		

Parameters of cubic spline polynomials (11.13.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	208	129	0.608	7.74−2	0.31	7.55−3	5
sat	208	129	0.606	7.51−2	0.31	7.68−3	6

T/K	A_1	A_2	A_3	A_4	Uncert.
180.4–250.0	3.782 35+1	−2.294 97+1	9.411 50	−1.120 03	II
250.0–330.0	1.838 86+1	3.722 08−1	8.274 02−2	1.238 01−1	III
330.0–463.1	3.665 59+1	−1.623 45+1	5.115 07	−3.845 15−1	IV
180.4–250.0	3.792 87+1	−2.308 87+1	9.471 85	−1.128 63	II
250.0–330.0	1.875 43+1	−7.937 75−2	2.681 19−1	9.853 29−2	III
330.0–463.1	4.862 00+1	−2.723 00+1	8.495 57	−7.325 23−1	IV

Deviation plot for Hexane (11-013) is given in Fig. 3.

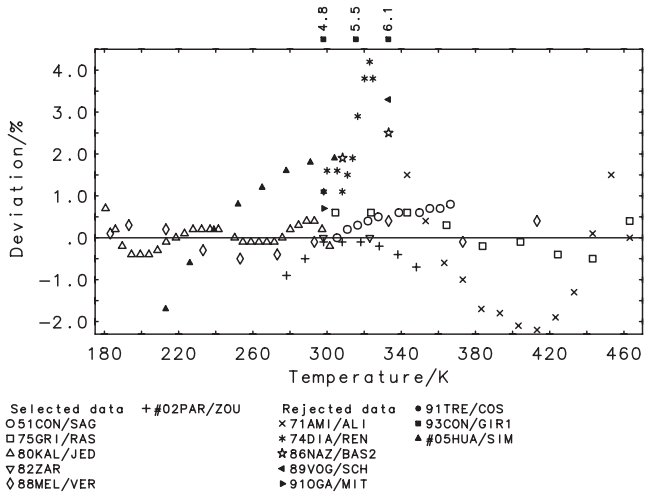

FIG. 3. Deviation plot for hexane (11-013).

6.2.1.3. Octane (11-032)

Name:	Octane
Formula:	C_8H_{18}
CAS-RN:	111-65-9
Group No:	11-032

Experimental heat capacities (11.32.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	344.9	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1930PAR/HUF2		223.0–293.7	8		n/a	n/a	n/a	*p*	BSIO	1925PAR
1931HUF/PAR		227.0–298.3	5		n/a	n/a	n/a	*p*	BSIO	1925PAR
1947OSB/GIN		285.6–305.6	5	S	0.10	99.96	estim	sat	BSAO	1947OSB/GIN
1949TSC/WET		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1951CON/SAG		299.8–366.5	13	S	n/a	n/a	n/a	*p*	BSAO	1939SAG/EVA
1954FIN/GRO2	N	222.6–297.6	18		0.20	99.94	melpt	sat	BSAO	1943RUE/HUF
1961ROU		283.1–312.3	15		n/a	99.83	anal	*p*	BSAO	1961ROU
1970AKH		293.1	1		n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
1971AMI/ALI	N	403.1–567.2	21	S	2.00	n/a	n/a	*p*	n/a	n/a
1975GRI/RAS	N	303.9–462.1	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1977NAZ/MUS		303.2–383.2	5		1.50	n/a	n/a	*p*	BSAO	1977NAZ/MUS
1980SHA/LYU		216.4–300.0	12	S	0.50	99.57	melpt	*p*	BSAO	1980SHA/LYU
1981GRO/ING		298.1	1		n/a	99.0	chrom	*p*	FSIT	1971PIC/LED
1982ZAR		298.0–363.0	3		0.60	n/a	n/a	*p*	BDCT	1982ZAR
1984GRI/AND	N	297.5–386.1	7		0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1984ROU/GRO		298.1	1		0.30	99.	estim	*p*	FSIT	1971PIC/LED
1985COS/PAT2		298.2	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985LAI/GRO		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1985LAI/ROD		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1986BEN/DAR1		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1991BAN/GAR		318.1–373.1	12		0.40	98.8	chrom	*p*	BDCT	1991BAN/GAR
1991OGA/MIT		298.1	1		n/a	n/a	n/a	*p*	FSIO	1985OGA
1991SOE/NAK		298.1	1		n/a	99.99	chrom	*p*	FSIO	1985OGA
1991TRE/COS		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992LAI/ROD		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993CZA1		298.8	1	2.00	n/a	n/a	*p*	BSIO	1979CZA
1995LAI/LOP		298.1	1	n/a	99.9	chrom	*p*	FSIT	1971PIC/LED
1999BUR/ZOC		298.1–323.1	2	2.00	n/a	n/a	*p*	FSIO	1999BUR/ZOC
1999TAM/OSA		298.1	1	n/a	99.99	anal	*p*	FSIO	1985OGA
2001CER/TOV2		288.1–333.1	5	n/a	99.5	chrom	*p*	BDHT	1969PER/COM
2005HUA/SIM		217.0–308.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN
2005PAR/TOV		288.1–308.1	3	n/a	99.5	anal	*p*	BDCT	1983ROU/ROU

Reference	Notes
1898LOU	average value in the temperature range 294–396 K
1954FIN/GRO2	smoothed data in 1967MES/GUT
1971AMI/ALI	calculated from C_v measured at the saturation line
1975GRI/RAS	grade: pure; the last five values at pressures higher than vapor pressure
1984GRI/AND	grade: pure

6.2.1.4. 2,2,4-Trimethylpentane (11-034)

Name:	2,2,4-Trimethylpentane
Formula:	C_8H_{18}
CAS-RN:	540-84-1
Group No:	11-034

Experimental heat capacities (11.34.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930PAR/HUF2		169.6–295.2	15		1.00	n/a	n/a	*p*	BSIO	1925PAR
1940PIT2		171.1–317.3	8		0.20	99.99	melpt	*p*	BSIO	1928LAT/GRE
1947OSB/GIN		285.6–305.6	5	S	0.10	99.96	melpt	sat	BSAO	1947OSB/GIN
1949TSC/WET		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1950AUE/SAG		299.8–366.5	13		1.00	99.9	melpt	*p*	BSAO	1939SAG/EVA
1961ROU		300.4–315.4	12		n/a	99.99	anal	*p*	BSAO	1961ROU
1973SUB/RAJ	N	298.1–323.1	3		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1976FOR/BEN1		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1984FIL/LAU		293.0	1		2.00	n/a	n/a	*p*	BDHO	1984FIL/LAU
1987KAL/KOH		293.1–313.1	2		n/a	99.98	chrom	*p*	FSIT	1971PIC/LED
1988COS/VAN		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1988SHI/OGA1		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA
1994BEN/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1995LAI/LOP		298.1	1		n/a	99.9	chrom	*p*	FSIT	1971PIC/LED
1999PIN/BRA		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
2000TAK/TAM		298.1	1		n/a	99.99	chrom	*p*	FSIO	1985OGA

Reference	Notes
1973SUB/RAJ	Same data in 1974RAJ/SUB

6.2.1.5. Nonane (11-038)

Name:	Nonane
Formula:	C_9H_{20}
CAS-RN:	111-84-2
Group No:	11-038

Experimental heat capacities (11.38.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930PAR/HUF2		224.5–299.1	8		1.00	n/a	n/a	*p*	BSIO	1925PAR
1931HUF/PAR		228.3–297.9	8		1.00	n/a	n/a	*p*	BSIO	1925PAR
1947OSB/GIN		283.1–313.1	4	S	0.10	99.96	estim	sat	BSAO	1947OSB/GIN
1954FIN/GRO2	N	225.0–313.9	22		0.20	99.88	melpt	sat	BSAO	1943RUE/HUF
1958SWI/ZIE1	N	348.8	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1970AKH		293.1	1		n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
1976MUS		307.8–417.8	10		2.50	n/a	n/a	*p*	BDAO	1971MUS
1979GRO/HAM		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1982WIL/ING		298.1	1		n/a	99.0	estim	*p*	FSIT	1971PIC/LED
1982ZAR		323.0–363.0	2		0.60	n/a	n/a	*p*	BDCT	1982ZAR
1988AND/PAT		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1991BAN/GAR		318.1–373.1	12		0.40	99.8	chrom	*p*	BDCT	1991BAN/GAR
1991OGA/MIT		298.1	1		n/a	n/a	n/a	*p*	FSIO	1985OGA
1991TRE/COS		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1997TOV/CAR4		288.1–308.1	3		n/a	99.0	anal	*p*	BDCT	1983ROU/ROU
2005HUA/SIM		220.0–313.0	eqn		n/a	99.0	error	*p*	BDHT	1999MO/YAN
2005PAR/TOV		288.1–308.1	3		n/a	99.0	anal	*p*	BDCT	1983ROU/ROU

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT
1958SWI/ZIE1	average value in the temperature range 295–402 K

6.2.1.6. Decane (11-041)

Name:	Decane
Formula:	$C_{10}H_{22}$
CAS-RN:	124-18-5
Group No:	11-041

Experimental heat capacities (11.41.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	360.9	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1930PAR/HUF2		242.3–295.5	6		1.00	n/a	n/a	*p*	BSIO	1925PAR
1931HUF/PAR		251.2–297.7	6		1.00	n/a	n/a	*p*	BSIO	1925PAR
1947OSB/GIN		290.6–305.6	4	S	0.10	99.96	estim	sat	BSAO	1947OSB/GIN
1952SCH/SAG		299.8–366.5	13	S	1.00	99.7	estim	sat	BSAO	1939SAG/EVA
1954FIN/GRO2	N	247.0–318.6	17		0.20	99.91	melpt	sat	BSAO	1943RUE/HUF
1970AKH		293.1	1		n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
1975GRI/RAS	N	303.3–462.4	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1979GRO/HAM		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1982PFE/KUC		298.1	1		n/a	n/a	n/a	*p*	BDCT	1968WAD
1982WIL/ING		298.1	1		n/a	99.0	estim	*p*	FSIT	1971PIC/LED
1982ZAR		298.0–363.0	3		0.60	n/a	n/a	*p*	BDCT	1982ZAR
1983SID/SVE		293.1	1		n/a	99.9	melpt	*p*	FSIT	1971PIC/LED
1984GRO/ING		298.1	1		n/a	99.0	melpt	*p*	FSIT	1971PIC/LED
1984ROU/GRO		298.1	1		n/a	98.0	estim	*p*	FSIT	1971PIC/LED
1985BAL/BRA		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985COS/PAT3		298.2	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985COS/PAT8		283.1–313.1	3		n/a	99.	estim	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1985LAI/ROD		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1985LAI/WIL		298.1	1	0.30	99.	estim	*p*	FSIT	1971PIC/LED
1986GAT/WOO		298.1–368.1	4	n/a	99.	anal	*p*	BDCT	1983ROU/ROU
1987WIL/ING		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1988COS/VAN		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1988KUZ/KHA		293.8–335.2	15	n/a	99.8	chrom	*p*	FSIO	1975SAF/GER
1988KUZ/KHA		310.1–421.9	16	n/a	n/a	n/a	*p*	FSIO	1975SAF/GER
1988PIN/BRA		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1991BAN/GAR		318.1–373.1	12	0.40	98.9	chrom	*p*	BDCT	1991BAN/GAR
1991TRE/COS		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992LAI/ROD		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1993CZA2		298.9	1	2.00	n/a	n/a	*p*	BSIO	1979CZA
1994JIM/ROM		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1996ROU/HER		298.1	1	n/a	98.	anal	*p*	FSIT	1971PIC/LED
1998BES/SAI	N	302.8–372.3	8	1.00	n/a	n/a	*p*	BDCT	2000BES/SAI2
2002CER/TOV		278.1–335.6	24	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2002PAR/ZOU		278.1–348.1	15	n/a	99.0	chrom	sat	BDCT	1983ROU/ROU
2002PEL/GON		280.1–318.1	5	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2005HUA/SIM		247.0–310.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN
2005PEL/TRO		283.1–303.1	5	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2005VAL/TRO		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1898LOU	average value in the temperature range 295–427 K
1954FIN/GRO2	smoothed data in 1967MES/GUT
1975GRI/RAS	last two values at pressures above the vapor pressure
1998BES/SAI	mixture data at elevated pressures

Correlated heat capacities (11.41.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	247.0–318.6	17	0.20		0.171	1.28−2	0.03	7.48−3	10
1975GRI/RAS	303.3–462.4	9	1.00		0.680	2.86−1	0.68	−8.25−2	−1
1982ZAR	298.0–363.0	3	0.60		0.946	2.26−1	0.57	−2.11−1	−3
1984GRO/ING	298.1	1	0.50	#	0.264	4.99−2	0.13	−4.99−2	−1
1984ROU/GRO	298.1	1	0.50	#	0.086	1.62−2	0.04	−1.62−2	−1
1985LAI/ROD	298.1	1	0.30	#	1.443	1.63−1	0.43	−1.63−1	−1
1986GAT/WOO	298.1–368.1	4	0.30	#	1.053	1.27−1	0.32	−1.26−1	−4
1988KUZ/KHA	293.8–335.2	15	0.50	#	0.455	8.74−2	0.23	8.08−2	15
1988KUZ/KHA	310.1–421.9	16	0.50	#	0.405	8.66−2	0.20	4.25−2	5
1991BAN/GAR	318.1–373.1	12	0.40		0.355	5.98−2	0.14	2.51−2	2
1993CZA2	298.9	1	2.00		0.039	2.95−2	0.08	−2.95−2	−1
1994JIM/ROM	298.1	1	0.50	#	0.622	1.17−1	0.31	−1.17−1	−1
1996ROU/HER	298.1	1	0.30	#	0.994	1.12−1	0.30	−1.12−1	−1?
1998BES/SAI	302.8–372.3	8	1.00		0.206	8.19−2	0.21	−6.87−2	−6
2002CER/TOV	278.1–335.6	24	0.40	#	0.201	3.04−2	0.08	8.52−3	4
2002PAR/ZOU	278.1–348.1	15	0.30	#	0.557	6.33−2	0.17	1.34−2	2
2002PEL/GON	280.1–318.1	5	0.30	#	0.125	1.41−2	0.04	2.35−3	0
2005HUA/SIM	247.0–310.0	6	1.00	#	0.599	2.14−1	0.60	−1.76−1	−6
2005PEL/TRO	283.1–303.1	5	0.30	#	0.797	8.98−2	0.24	−8.83−2	−5
2005VAL/TRO	288.1–308.1	3	0.30	#	0.693	7.95−2	0.21	7.20−2	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1898LOU	(4.07−1, 0.96, 4.07−1, 1)	1930PAR/HUF2	(6.51−1, 1.83, −6.12−1, −5)
1931HUF/PAR	(3.02−1, 0.83, −2.98−1, −6)	1947OSB/GIN	(3.27−1, 0.86, −1.84−2, 0)
1952SCH/SAG	(3.98−1, 1.02, −3.59−1, −11)	1970AKH	(4.42−1, 1.19, −4.42−1, −1)
1979GRO/HAM	(1.26−1, 0.33, −1.26−1, −1)	1982PFE/KUC	(2.61−1, 0.70, −2.61−1, −1)
1982WIL/ING	(2.19−1, 0.58, −2.19−1, −1)	1983SID/SVE	(2.16−1, 0.58, −2.16−1, −1)
1985BAL/BRA	(1.33−1, 0.35, −1.33−1, −1)	1985COS/PAT3	(1.31−1, 0.35, 1.31−1, 1)
1985COS/PAT8	(1.55−1, 0.41, 5.12−2, 1)	1985LAI/WIL	(1.51−1, 0.40, −1.51−1, −1)
1987WIL/ING	(1.71−1, 0.46, −1.71−1, −1)	1988COS/VAN	(1.17−1, 0.31, 1.17−1, 1)
1988PIN/BRA	(1.46−1, 0.39, −1.46−1, −1)	1991TRE/COS	(1.34−1, 0.35, 1.34−1, 1)
1992LAI/ROD	(2.10−1, 0.56, −2.10−1, −1)		

Parameters of cubic spline polynomials (11.41.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	194	148	0.497	1.11−1	0.28	−9.87−3	10
sat	194	148	0.498	1.11−1	0.28	−9.85−3	10

T/K	A_1	A_2	A_3	A_4	Uncert.
247.0–314.0	8.691 77+1	−5.471 10+1	1.824 88+1	−1.818 98	II
314.0–462.4	3.281 32+1	−3.018 91	1.786 33	−7.137 39−2	III
247.0–314.0	8.648 27+1	−5.425 34+1	1.808 91+1	−1.800 49	II
314.0–462.4	3.401 59+1	−4.125 88	2.124 88	−1.057 73−1	III

Deviation plot for Decane is given in Fig. 4.

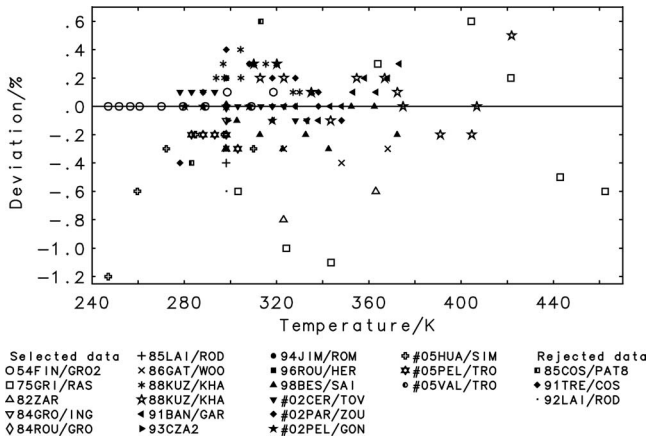

FIG. 4. Deviation plot for decane (11-041).

6.2.1.7. Undecane (11-048)

Name:	Undecane
Formula:	$C_{11}H_{24}$
CAS-RN:	1120-21-4
Group No:	11-048

Experimental heat capacities (11.48.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931HUF/PAR		258.5–298.0	4	1.00	n/a	n/a	*p*	BSIO	1925PAR
1954FIN/GRO2	N	251.7–298.9	12	0.20	99.98	melpt	sat	BSAO	1943RUE/HUF
1970AKH		293.1	1	n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
1976MUS		307.8–458.6	14	2.50	n/a	n/a	*p*	BDAO	1971MUS
1984GRI/AND		292.3–433.4	8	0.80	n/a	n/a	*p*	BSAO	1967RAS/GAN
2005HUA/SIM		248.0–313.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN
2005PEL/TRO		283.1–303.1	5	n/a	99.0	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT

6.2.1.8. Dodecane (11-049)

Name:	Dodecane
Formula:	$C_{12}H_{26}$
CAS-RN:	112-40-3
Group No:	11-049

Experimental heat capacities (11.49.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931HUF/PAR		275.1–297.7	4	1.00	n/a	n/a	*p*	BSIO	1925PAR
1954FIN/GRO2	N	266.7–317.4	11	0.20	99.93	melpt	sat	BSAO	1943RUE/HUF
1971REC/SAD		303.1	1	0.30	n/a	n/a	*p*	BSIO	1970REC
1973KAL/WOY		303.1	1	0.20	99.5	chrom	*p*	BSIO	1970REC
1977NAZ/MUS		303.2–483.2	10	1.50	n/a	n/a	*p*	BSAO	1977NAZ/MUS
1981GRO/ING		298.1	1	n/a	99.0	chrom	*p*	FSIT	1971PIC/LED
1982ZAR		298.0–363.0	3	0.60	n/a	n/a	*p*	BDCT	1982ZAR
1984GRO/BEN		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1984KUM/BEN		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1984ROU/GRO		298.1	1	n/a	98.	estim	*p*	FSIT	1971PIC/LED
1985BEN/KUM		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985COS/PAT4		298.2	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985COS/PAT8		283.1–313.1	3	n/a	99.0	estim	*p*	FSIT	1971PIC/LED
1985LAI/ROD		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1986BEN/DAR3		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1986WIL/LAI		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1988AND/PAT		298.1	1	n/a	98.	anal	*p*	FSIT	1971PIC/LED
1988COS/VAN		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1989LAI/ROD		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1989VOG/SCH		333.1	1	n/a	n/a	n/a	*p*	BDHT	1969PER/COM
1991TRE/COS		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992LAI/ROD		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997TOV/CAR1		283.1–308.1	4	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
1998SAL/FER		293.0–370.0	eqn	n/a	99.	chrom	*p*	BDHT	1998SAL/FER
1999BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	1999BUR/ZOC
2001CER/TOV2		288.1–333.1	5	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2001PEL/GON		280.1–318.1	5	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2001PAR/TOV2		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2002GON/TOV	N	283.1–323.1	6	n/a	99.2	chrom	*p*	BDCT	1970PAZ/PAZ
2002PAR/ZOU		298.1–338.1	3	n/a	99.0	chrom	sat	BDCT	1983ROU/ROU
2004PEL/TRO		288.1–303.1	4	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2004TRO/VAL		288.1–318.1	4	n/a	99.2	chrom	*p*	BDHT	1969PER/COM
2005HUA/SIM		267.0–329.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT
2002GON/TOV	same data in 2004GON/PEL

Correlated heat capacities (11.49.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	266.7–317.4	11	0.20		0.214	1.93−2	0.04	1.07−2	8
1977NAZ/MUS	303.2–483.2	10	1.50		0.103	7.30−2	0.16	−1.92−3	−4
1981GRO/ING	298.1	1	0.50	#	0.535	1.21−1	0.27	−1.21−1	−1
1982ZAR	298.0–363.0	3	0.60		0.811	2.26−1	0.49	−1.56−1	−3
1984GRO/BEN	298.1	1	0.50	#	0.300	6.76−2	0.15	−6.76−2	−1
1984KUM/BEN	298.1	1	0.50	#	0.278	6.28−2	0.14	−6.28−2	−1
1985BEN/KUM	298.1	1	0.50	#	0.353	7.97−2	0.18	−7.97−2	−1
1985COS/PAT4	298.2	1	0.50	#	0.081	1.84−2	0.04	1.84−2	1
1985COS/PAT8	283.1–313.1	3	0.50	#	1.013	2.32−1	0.51	9.01−2	1
1986BEN/DAR3	298.1	1	0.50	#	0.241	5.44−2	0.12	−5.44−2	−1
1988AND/PAT	298.1	1	0.50	#	0.339	7.67−2	0.17	7.67−2	1
1988COS/VAN	298.1	1	0.50	#	0.142	3.22−2	0.07	3.22−2	1
1991TRE/COS	298.1	1	0.50	#	0.094	2.14−2	0.05	2.14−2	1
1997TOV/CAR1	283.1–308.1	4	0.50	#	0.463	1.05−1	0.23	1.02−1	4
1998SAL/FER	293.0–370.0	8	0.50	#	0.643	1.49−1	0.32	−1.04−1	−4
2001CER/TOV2	288.1–333.1	5	0.50	#	0.466	1.10−1	0.23	9.09−2	5
2001PEL/GON	280.1–318.1	5	0.50	#	0.068	1.52−2	0.03	1.01−2	3
2001PAR/TOV2	288.1–308.1	3	0.50	#	0.263	5.94−2	0.13	5.83−2	3
2002GON/TOV	283.1–323.1	6	0.50	#	0.417	9.49−2	0.21	−9.40−2	−6
2002PAR/ZOU	298.1–338.1	3	0.50	#	0.154	3.64−2	0.08	2.68−2	1
2004PEL/TRO	288.1–303.1	4	0.50	#	0.252	5.69−2	0.13	−5.60−2	−4
2004TRO/VAL	288.1–318.1	4	0.50	#	0.068	1.53−2	0.03	8.27−3	2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1931HUF/PAR	(3.79−1, 0.86, −3.70−1, −4)	1971REC/SAD	(4.26−1, 0.95, −4.26−1, −1)
1973KAL/WOY	(9.17−1, 2.06, −9.17−1, −1)	1984ROU/GRO	(1.07−1, 0.24, −1.07−1, −1)
1985LAI/ROD	(3.03−1, 0.68, −3.03−1, −1)	1986WIL/LAI	(3.03−1, 0.68, −3.03−1, −1)
1989LAI/ROD	(4.45−1, 01.00, −4.45−1, −1)	1989VOG/SCH	(1.32, 2.70, 1.32, 1)
1992LAI/ROD	(3.45−1, 0.77, −3.45−1, −1)	1999BUR/ZOC	(8.16−1, 1.76, 7.68−1, 2)
2005HUA/SIM	(2.14−1, 0.49, −1.22−1, −2)		

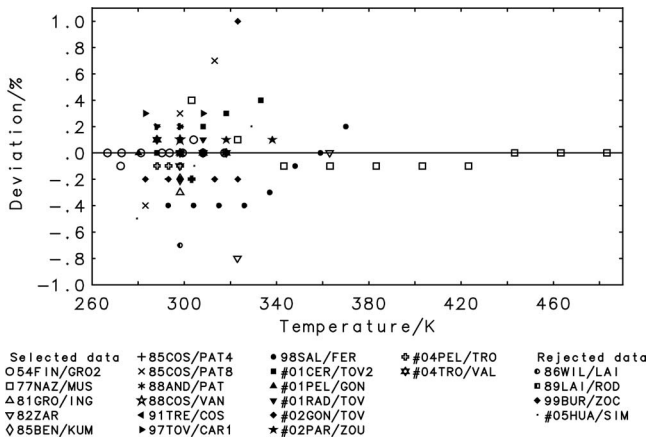

FIG. 5. Deviation plot for dodecane (11-049).

Parameters of cubic spline polynomials (11.49.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	98	78	0.427	1.03−1	0.22	−9.59−3	5
sat	98	78	0.427	1.03−1	0.22	−9.49−3	5

T/K	A_1	A_2	A_3	A_4	Uncert.
266.7–310.0	1.772 10+2	−1.363 08+2	4.489 39+1	−4.704 43	II
310.0–483.2	3.073 15+1	5.445 70	−8.330 98−1	2.124 48−1	IV
266.7–310.0	1.765 41+2	−1.356 25+2	4.466 18+1	−4.678 22	II
310.0–483.2	3.135 73+1	4.875 80	−6.608 96−1	1.951 90−1	IV

Deviation plot for Dodecane is given in Fig. 5.

6.2.1.9. Tridecane (11-051)

Name:	Tridecane
Formula:	$C_{13}H_{28}$
CAS-RN:	629-50-5
Group No:	11-051

Experimental heat capacities (11.51.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1954FIN/GRO2	N	271.7–306.4	8	0.20	99.95	melpt	sat	BSAO	1943RUE/HUF
1975WOY/KAL		303.1	1	n/a	99.97	chrom	p	BSIO	1970REC
1976MUS		307.8–478.6	16	2.50	n/a	n/a	p	BDAO	1971MUS
2000BES/SAI1	N	313.1–373.1	7	1.00	99.0	anal	p	BDCT	2000BES/SAI2
2001PEL/GON		280.1–318.1	5	n/a	99.0	chrom	p	BDHT	1969PER/COM
2004PEL/TRO		298.1–303.1	2	n/a	99.0	chrom	p	BDHT	1969PER/COM
2005HUA/SIM		269.0–319.0	eqn	n/a	99.0	error	p	BDHT	1999MO/YAN

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT
2000BES/SAI1	data at elevated pressures

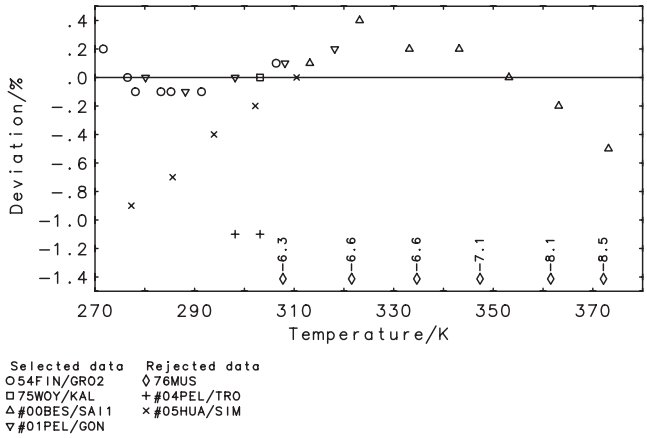

FIG. 6. Deviation plot for tridecane (11-051).

Correlated heat capacities (11.51.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	271.7–306.4	8	0.20		0.553	5.33−2	0.11	−2.30−3	−4
1975WOY/KAL	303.1	1	0.50	#	0.088	2.16−2	0.04	2.16−2	1
2000BES/SAI1	313.1–373.1	7	1.00		0.286	1.51−1	0.29	1.32−2	3
2001PEL/GON	280.1–318.1	5	0.50	#	0.184	4.59−2	0.09	1.55−2	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1976MUS	(3.53, 7.24, −3.49, −6)	2004PEL/TRO	(5.41−1, 1.12, −5.41−1, −2)
2005HUA/SIM	(2.43−1, 0.51, −1.52−1, −2)		

Parameters of regression polynomial (11.51.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	46	21	0.422	1.04−1	0.20	8.24−3	0

T/K	A_1	A_2	A_3	A_4	Uncert.
271.7–373.1	5.560 85+1	−9.934 89	2.581 83		III

Deviation plot for Tridecane is given in Fig. 6.

6.2.1.10. Tetradecane (11-052)

Name:	Tetradecane
Formula:	$C_{14}H_{30}$
CAS-RN:	629-59-4
Group No:	11-052

Experimental heat capacities (11.52.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1934PAR/LIG		280.6–290.6	4	1.00	n/a	n/a	*p*	BSIO	1925PAR
1954FIN/GRO2	N	282.7–302.8	7	0.20	99.93	melpt	sat	BSAO	1943RUE/HUF
1976MUS		307.8–501.5	18	2.50	n/a	n/a	*p*	BDAO	1971MUS
1982ZAR		298.0–363.0	3	0.60	n/a	n/a	*p*	BDCT	1982ZAR
1984GRI/AND		296.2–433.3	8	0.80	n/a	n/a	*p*	BSAO	1967RAS/GAN
1984GRO/BEN		298.1	1	n/a	99.5	estim	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1984GRO/ING		298.1	1	n/a	99.	estim	p	FSIT	1971PIC/LED
1984ROU/GRO		298.1	1	n/a	99.	estim	p	FSIT	1971PIC/LED
1985BAL/BRA		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1985LAI/WIL		298.1	1	0.30	99.5	estim	p	FSIT	1971PIC/LED
1986WIL/LAI		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1987WIL/ING		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1988COS/VAN		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1991TRE/COS		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1992LAI/ROD		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1995LAI/LOP		298.1	1	n/a	99.9	chrom	p	FSIT	1971PIC/LED
1995WIL/ING		298.1	1	n/a	99.0	chrom	p	FSIT	1971PIC/LED
1996ROU/HER		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
2000TOV/CER		288.1–308.1	4	n/a	99.0	chrom	p	BDHT	1969PER/COM
2001PAR/TOV2		288.1–308.1	3	n/a	99.0	chrom	p	BDHT	1969PER/COM
2005HUA/SIM		286.0–318.0	eqn	n/a	99.0	error	p	BDHT	1999MO/YAN

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT

Correlated heat capacities (11.52.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	282.7–302.8	7	0.20		0.200	2.12−2	0.04	1.27−2	3
1982ZAR	298.0–363.0	3	0.60		0.793	2.69−1	0.48	1.21−2	−1
1984GRI/AND	296.2–433.3	8	0.80		0.412	1.88−1	0.33	−1.19−1	−6
1984ROU/GRO	298.1	1	0.50	#	0.624	1.64−1	0.31	−1.64−1	−1
1988COS/VAN	298.1	1	0.50	#	0.120	3.15−2	0.06	−3.15−2	−1
1991TRE/COS	298.1	1	0.50	#	0.004	9.35−4	0.00	9.35−4	0
2000TOV/CER	288.1–308.1	4	1.00	#	0.116	6.21−2	0.12	4.62−2	4
2001PAR/TOV2	288.1–308.1	3	1.00	#	0.126	6.69−2	0.13	5.93−2	3
2005HUA/SIM	294.0–318.0	4	1.00	#	0.266	1.39−1	0.27	−9.29−2	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1934PAR/LIG	(9.56−2, 0.18, −9.54−2, −3)	1976MUS	(5.91, 11.17, −5.83, −11)
1984GRO/BEN	(2.25−1, 0.43, −2.25−1, −1)	1984GRO/ING	(2.11−1, 0.40, −2.11−1, −1)
1985BAL/BRA	(5.70−1, 1.09, −5.70−1, −1)	1985LAI/WIL	(4.90−1, 0.94, −4.90−1, −1)
1986WIL/LAI	(5.16−1, 0.99, −5.16−1, −1)	1987WIL/ING	(4.95−1, 0.95, −4.95−1, −1)
1992LAI/ROD	(5.97−1, 1.14, −5.97−1, −1)	1995LAI/LOP	(4.45−1, 0.85, −4.45−1, −1)
1995WIL/ING	(6.76−1, 1.27, 6.76−1, 1)	1996ROU/HER	(3.03−1, 0.58, −3.03−1, −1)

Parameters of cubic spline polynomials (11.52.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	65	32	0.400	1.54−1	0.28	−3.23−2	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
282.7–310.0	−2.834 27+1	7.867 07+1	−2.723 48+1	3.342 84	II
310.0–433.3	1.288 38+2	−7.343 98+1	2.183 31+1	−1.933 28	IV

Deviation plot for Tetradecane is given in Fig. 7.

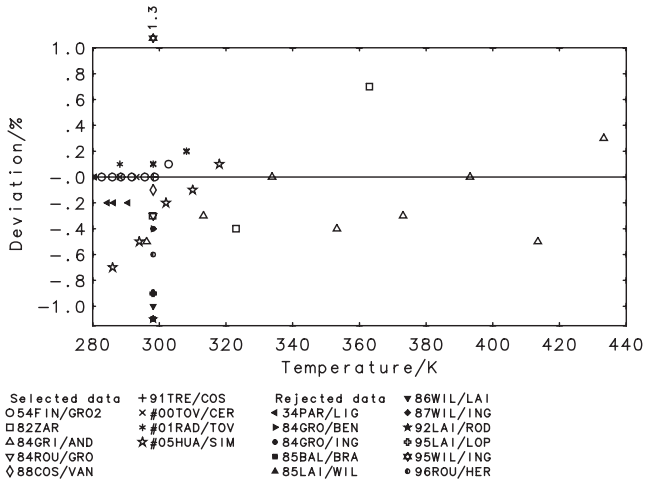

FIG. 7. Deviation plot for tetradecane (11-052).

6.2.1.11. Pentadecane (11-053)

Name:	Pentadecane
Formula:	$C_{15}H_{32}$
CAS-RN:	629-62-9
Group No:	11-053

Experimental heat capacities (11.53.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1954FIN/GRO2	N	285.5–312.8	7	0.20	99.95	melpt	sat	BSAO	1943RUE/HUF
1970AKH		293.1	1	n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
1981GRO/ING		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1988COS/VAN		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1991TRE/COS		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
2001BES/SAI	N	313.1–373.1	7	1.00	99.0	anal	*p*	BDCT	2000BES/SAI2
2005HUA/SIM		284.0–319.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT
2001BES/SAI	data at elevated pressures up to 100 MPa

Correlated heat capacities (11.53.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	285.5–312.8	7	0.20		0.090	1.01−2	0.02	−9.62−4	0
1991TRE/COS	298.1	1	0.50	#	0.201	5.69−2	0.10	5.69−2	1
2001BES/SAI	313.1–373.1	7	1.00		0.040	2.42−2	0.04	−8.65−3	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1970AKH	(7.09−1, 1.25, 7.09−1, 1)	1981GRO/ING	(2.64−1, 0.47, −2.64−1, −1)
1988COS/VAN	(1.44−1, 0.26, −1.44−1, −1)	2005HUA/SIM	(2.03−1, 0.36, −1.69−1, −4)

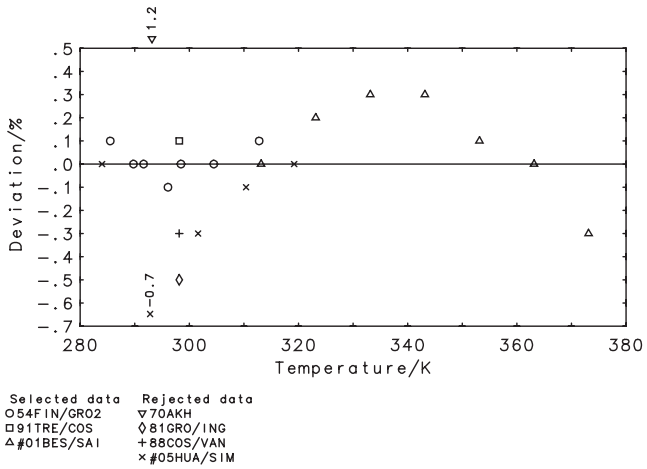

FIG. 8. Deviation plot for pentadecane (11-053).

Parameters of regression polynomial (11.53.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	23	15	0.099	2.70−2	0.05	−6.91−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
285.5–373.1	2.215 20+2	−1.579 19+2	4.836 76+1	−4.682 80	III

Parameters of quasipolynomial equation (11.53.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	23	15	0.310	1.31−1	0.22	3.44−2	4

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
285.5–373.1	708.00	8.124 13+1	4.907 99+1	2.027 45	3.361 94+1			III

Deviation plot for Pentadecane is given in Fig. 8.

6.2.1.12. Hexadecane (11-055)

Name:	Hexadecane
Formula:	$C_{16}H_{34}$
CAS-RN:	544-76-3
Group No:	11-055

Experimental heat capacities (11.55.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1949PAR/MOO		290.0–300.0	2	S	1.00	95.	estim	p	BSIO	1925PAR
1954FIN/GRO2	N	295.4–320.3	9		0.20	99.88	melpt	sat	BSAO	1943RUE/HUF
1956SCH/GOT		292.1–294.6	4		2.00	n/a	n/a	p	BSAO	1933SOU/BRI
1962GOL/BEL		310.9–422.0	3		n/a	96.9	chrom	p	BDHT	1963GUD/CAM
1968REC1	N	298.0–313.0	eqn		n/a	n/a	n/a	p	BSAO	1968REC1
1970AKH		293.1	1		n/a	n/a	n/a	p	BDHO	1959ABA/MUS
1971REC/SAD		303.1	1		0.30	n/a	n/a	p	BSIO	1970REC
1972REC/SAD		298.1	1		0.30	n/a	n/a	p	BSIO	1970REC
1973KAL/WOY		303.1	1		0.20	99.5	chrom	p	BSIO	1970REC

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1974DIA/REN		300.1–323.5	9	0.30	n/a	n/a	*p*	BSAO	1974DIA/REN
1974PET/TER		297.8–453.5	14	1.00	98.	melpt	*p*	BDCT	1974PET/TER
1981GRO/ING		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1982PFE/KUC		298.1	1	n/a	n/a	n/a	*p*	BDCT	1968WAD
1982ZAR		298.0–363.0	3	0.60	n/a	n/a	*p*	BDCT	1982ZAR
1985COS/PAT5		298.2	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1985LAI/ROU		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1986WIL/LAI		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1988COS/VAN		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1989LAI/ROD		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1991BAN/GAR		318.1–373.1	12	0.40	99.4	chrom	*p*	BDCT	1991BAN/GAR
1991TRE/COS		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992LAI/ROD		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1994BEN/ROU		298.1	1	n/a	98.	anal	*p*	FSIT	1971PIC/LED
2001CER/TOV2		308.1–333.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2005HUA/SIM		295.0–328.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1954FIN/GRO2	smoothed data in 1967MES/GUT
1968REC1	same data in 1968REC3

Correlated heat capacities (11.55.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1954FIN/GRO2	295.4–320.3	9	0.20		0.303	3.72−2	0.06	1.82−2	2
1970AKH	293.1	1	3.00	#	0.078	1.41−1	0.23	1.41−1	1
1973KAL/WOY	303.1	1	0.20		0.501	6.08−2	0.10	6.08−2	1
1974DIA/REN	300.1–323.5	9	0.30		0.601	1.11−1	0.18	2.71−2	5
1974PET/TER	297.8–453.5	14	1.00		0.800	5.10−1	0.80	−1.19−1	−4
1981GRO/ING	298.1	1	0.50	#	0.604	1.82−1	0.30	−1.82−1	−1
1982ZAR	298.0–363.0	3	0.60		1.276	4.85−1	0.77	−8.53−2	−1
1988COS/VAN	298.1	1	0.50	#	0.507	1.53−1	0.25	−1.53−1	−1
1991BAN/GAR	318.1–373.1	12	0.40		0.390	1.00−1	0.16	−5.91−2	−8
1991TRE/COS	298.1	1	0.50	#	0.704	2.12−1	0.35	−2.12−1	−1
2001CER/TOV2	308.1–333.1	3	0.50	#	0.211	6.61−2	0.11	5.75−2	3
2005HUA/SIM	295.0–328.2	5	1.00	#	0.286	1.77−1	0.29	4.79−2	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1949PAR/MOO	(3.10−1, 0.51, 3.10−1, 1)	1956SCH/GOT	(3.34, 5.26, 3.33, 2)
1962GOL/BEL	(2.03, 3.36, −1.85, −3)	1968REC1	(2.03−1, 0.33, −1.86−1, −3)
1971REC/SAD	(6.70−1, 1.12, −6.70−1, −1)	1972REC/SAD	(5.87−1, 0.98, −5.87−1, −1)
1982PFE/KUC	(8.60−1, 1.45, −8.60−1, −1)	1985COS/PAT5	(2.27−1, 0.38, −2.27−1, −1)
1985LAI/ROU	(6.05−1, 1.01, −6.05−1, −1)	1986WIL/LAI	(6.92−1, 1.16, −6.92−1, −1)
1989LAI/ROD	(5.20−1, 0.87, −5.20−1, −1)	1992LAI/ROD	(6.42−1, 1.08, −6.42−1, −1)
1994BEN/ROU	(6.47−1, 1.08, −6.47−1, −1)		

Parameters of cubic spline polynomials (11.55.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	81	60	0.628	2.98−1	0.47	−3.60−2	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
293.1–350.0	1.694 84+2	−1.069 95+2	3.291 66+1	−3.122 99	II
350.0–453.6	9.882 61+1	−4.643 13+1	1.561 26+1	−1.474 99	V

Parameters of quasipolynomial equation (11.55.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	81	60	0.762	3.20−1	0.51	−6.17−2	−22

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
293.1–453.5	722.00	2.497 09	2.513 86−2	3.589 02+1	6.201 07+1			IV

Deviation plot for Hexadecane is given in Fig. 9.

6.2.1.13. Heptadecane (11-056)

Name:	Heptadecane
Formula:	$C_{17}H_{36}$
CAS-RN:	629-78-7
Group No:	11-056

Experimental heat capacities (11.56.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1967MES/GUT		301.9–384.4	11	0.10	99.89	melpt	sat	BSAO	1947HUF
1970AKH		293.1	1	n/a	n/a	n/a	*p*	BDHO	1959ABA/MUS
2000VAN		299.0–401.1	46	0.20	99.	anal	*p*	BSAO	1998VAN/VAN
2005HUA/SIM		301.0–328.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

6.2.1.14. Octadecane (11-057)

Name:	Octadecane
Formula:	$C_{18}H_{38}$
CAS-RN:	593-45-3
Group No:	11-057

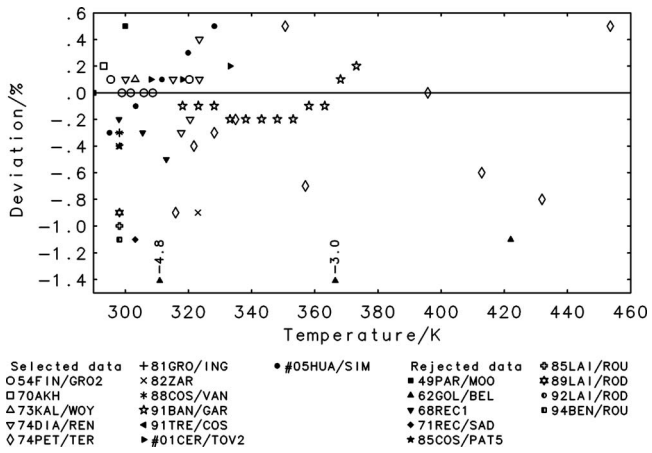

FIG. 9. Deviation plot for hexadecane (11-055).

Experimental heat capacities (11.57.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1949PAR/MOO		300.0	1		1.00	96.	estim	*p*	BSIO	1925PAR
1967MES/GUT		304.4–378.7	11		0.10	99.98	melpt	sat	BSAO	1947HUF
1981HOE		325.0–375.0	3	S	5.00	n/a	n/a	*p*	BDHT	1969PER/COM
1983MEY/MEY	N	303.0	1		n/a	99.5	melpt	*p*	BSIO	1983MEY/MEY
1986DJO/LAU	N	315.0	1		n/a	n/a	n/a	*p*	BDHT	1969PER/COM
1993DUR/AOU	N	373.0–473.0	51		n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
2000VAN		306.7–401.1	38		0.20	99.8	anal	*p*	BSAO	1998VAN/VAN
2005HUA/SIM		305.0–329.0	eqn		n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1983MEY/MEY	in the article temperature is unspecified; probably above melting temperature
1986DJO/LAU	very suspect value
1993DUR/AOU	an equation in 1996DUR/AOU

6.2.1.15. Nonadecane (11-058)

Name:	Nonadecane
Formula:	$C_{19}H_{40}$
CAS-RN:	629-92-5
Group No:	11-058

Experimental heat capacities (11.58.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1969ATK/LAR		305.0–453.0	eqn	n/a	99.9	chrom	*p*	BSAO	1958WES/GIN
1984GRI/AND		313.1–433.2	10	0.70	n/a	n/a	*p*	BSAO	1967RAS/GAN
1993DUR/AOU	N	373.0–473.0	51	n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1999VAN/OON		306.2–380.0	47	0.20	99.54	melpt	*p*	BSAO	1987VAN/VAN
2005HUA/SIM		306.0–329.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1993DUR/AOU	an equation in 1996DUR/AOU

6.2.2. Sub group 12: saturated cyclic hydrocarbons

6.2.2.1. Cyclohexane (12-007)

Name:	Cyclohexane
Formula:	C_6H_{12}
CAS-RN:	110-82-7
Group No:	12-007

Experimental heat capacities (12.7.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1919DEJ		295.6–323.3	10	n/a	n/a	n/a	*p*	BSIO	1919DEJ
1930PAR/HUF2		283.1–298.9	5	0.30	n/a	n/a	*p*	BSIO	1925PAR
1939PHI		304.1	1	n/a	n/a	n/a	*p*	BSIO	1949WEI
1943AST/SZA		281.6–292.5	4	n/a	99.905	melpt	*p*	BSAO	1939AST/EID1
1943RUE/HUF		282.3–301.3	7	0.10	99.985	melpt	*p*	BSAO	1943RUE/HUF
1948TSC2		292.6	1	n/a	n/a	n/a	*p*	BSIO	1948TSC1

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1948TSC6		293.6	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1950AUE/SAG		299.8–366.5	13		n/a	99.9	melpt	*p*	BSAO	1939SAG/EVA
1960SWI/ZIE	N	311.6–322.2	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1961ROU		300.4–315.8	7		n/a	99.94	anal	*p*	BSAO	1961ROU
1964MOE/THO		298.0–327.7	4		0.50	n/a	n/a	*p*	BSIO	1964MOE/THO
1966KLE		293.1–343.1	11	S	0.10	n/a	n/a	*p*	BSAO	1966KLE
1966NIK/RAB		283.1–333.1	11	S	0.30	n/a	n/a	*p*	BSAO	1947SKU
1968REC1	N	298.0–313.0	eqn		n/a	n/a	n/a	*p*	BSAO	1968REC1
1969WIL/SCH		293.1–313.1	3		0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1973SUB/RAJ		298.1–323.1	3		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1974WIL/ZET		283.1–323.1	5		n/a	n/a	n/a	*p*	BSAO	1964ARN1
1975JOL/BOI		298.1	1		0.30	99.9	melpt	*p*	FSIT	1971PIC/LED
1975SAN	N	398.1–523.2	9	S	1.00	n/a	n/a	*p*	FSIO	1975SAN
1978GRO/WIL		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1978SAF		299.1–311.7	7		0.30	n/a	n/a	*p*	BSAO	1967RAS/GAN
1978SAF		299.1–311.7	7		0.30	n/a	n/a	*p*	BSAO	1967RAS/GAN
1978SAF		299.1–311.7	7		n/a	n/a	n/a	*p*	BSAO	1967RAS/GAN
1979FOR/DAR		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1979MAR/BRA		298.1	1		1.00	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1979WIL/GRO		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1982GRO/ING		298.1	1		0.30	99.5	melpt	*p*	FSIT	1971PIC/LED
1982TAN		293.1–303.1	3	S	0.30	99.99	chrom	*p*	FSIT	1971PIC/LED
1983SID/SVE		293.1	1		0.30	99.9	chrom	*p*	FSIT	1971PIC/LED
1985NKI/CHA		298.0	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1985TAN/NAK		283.1–318.1	3		0.30	100	chrom	*p*	FSIT	1971PIC/LED
1986JIM/ROM		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1986ORT		298.1	1		1.00	99.5	anal	*p*	BDCT	1970PAZ/PAZ
1987KAL/KOH		293.1–313.1	2		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1988SHI/OGA2		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA
1989JIM/ROU		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1989LAI/ROD		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1990JAL/ROB		293.0	1		5.00	99.	anal	*p*	BDHT	1995DIO/MAN
1991OGA/MIT		298.1	1		n/a	n/a	n/a	*p*	FSIO	1985OGA
1991TRE/COS		298.1	1		n/a	99.98	anal	*p*	FSIT	1971PIC/LED
1994BEN/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994CON/GIA1		298.1	1		n/a	n/a	n/a	*p*	FSIT	1988CON/GIA
1994CON/GIA2		298.1	1		n/a	99.8	anal	*p*	FSIT	1988CON/GIA
1994LAI/WIL		298.1–298.1	2		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1995CON/GIA1		298.1	1		0.50	99.8	chrom	*p*	FSIT	1988CON/GIA
1995LOW/PEU		298.2	1		1.00	n/a	n/a	*p*	BDCO	1995LOW/PEU
1995TAK/OGA		298.1	1		1.00	99.99	chrom	*p*	FSIO	1985OGA
1997CON/GIA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1988CON/GIA
1997NIS/TAB		293.1–303.1	3		n/a	99.99	chrom	*p*	FSIO	1985OGA
1997TOV/CAR3		288.1–308.1	3		n/a	99.9	anal	*p*	BDCT	1983ROU/ROU
1998CON/GIA		298.1	1		0.50	99.5	chrom	*p*	FSIT	1988CON/GIA
1999BRO/CAL1		298.1	1		n/a	99.9	chrom	*p*	FSIT	1971PIC/LED
2000TOV/CER		288.1–308.1	4		n/a	99.9	chrom	*p*	BDHT	1969PER/COM
2001CER/TOV2		288.1–333.1	5		n/a	99.9	chrom	*p*	BDHT	1969PER/COM
2001PAR/TOV1		288.1–308.1	3		n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2002PAR/ZOU		288.1–348.1	7		n/a	99.5	chrom	sat	BDCT	1983ROU/ROU
2004NAN/TAN		283.6–339.9	19		0.40	99.9965	melpt	*p*	BSAO	1995TAN/SUN

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005HUA/SIM		283.0–303.0	eqn	n/a	99.0	error	*p*	BDHT	1999MO/YAN

Reference	Notes
1960SWI/ZIE	average values in the temperature ranges 294–329 and 294–350 K
1968REC1	same data in 1968REC2
1975SAN	same data in 1976SAN/MEL; C_p at the saturation pressure extrapolated from high pressure measurement

6.2.2.2. Methylcyclohexane (12-019)

Name:	Methylcyclohexane
Formula:	C_7H_{14}
CAS-RN:	108-87-2
Group No:	12-019

Experimental heat capacities (12.19.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930PAR/HUF1		151.4–294.2	12	1.00	n/a	n/a	*p*	BSIO	1925PAR
1946DOU/HUF1		155.1–285.8	15	0.10	99.989	melpt	*p*	BSAO	1943RUE/HUF
1948TSC2		292.6	1	n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC6		293.6	1	n/a	n/a	n/a	*p*	BSIO	1948TSC1
1966HWA/ZIE		174.8–308.1	32	n/a	99.0	melpt	*p*	BSAO	1945SCO/MEY
1975HOL/ZIE		144.0–312.0	eqn	0.20	99.88	anal	*p*	BSAO	1945SCO/MEY
1979WIL/GRO		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1982GRO/ING		298.1	1	0.30	99.5	estim	*p*	FSIT	1971PIC/LED
1983SID/SVE		293.1	1	0.30	99.9	chrom	*p*	FSIT	1971PIC/LED
1985TAN		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1988SHI/OGA2		298.1	1	n/a	99.9	chrom	*p*	FSIO	1985OGA
2000BEC/AUF		288.2–353.2	14	0.20	99.95	chrom	sat	BDCT	2000BEC/AUF
2000TAM/OSA		298.1	1	n/a	99.85	chrom	*p*	FSIO	1985OGA

6.2.2.3. Cyclooctane (12-028)

Name:	Cyclooctane
Formula:	C_8H_{16}
CAS-RN:	292-64-8
Group No:	12-028

Experimental heat capacities (12.28.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1956FIN/SCO		294.6–321.6	6	0.10	99.82	melpt	sat	BSAO	1943RUE/HUF
1975JOL/BOI		298.1	1	0.30	99.7	melpt	*p*	FSIT	1971PIC/LED
1979FOR/DAR		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1979WIL/FAR		298.1	1	0.30	99.0	melpt	*p*	FSIT	1971PIC/LED
1985TAN		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1988SHI/OGA2		298.1	1	n/a	99.9	chrom	*p*	FSIO	1985OGA
1995LAI/LOP		298.1	1	n/a	99.9	chrom	*p*	FSIT	1971PIC/LED

6.2.2.4. Octahydro-4,7-methano-1*H*-indene (12-047)

Name:	Octahydro-4,7-methano-1*H*-indene
Formula:	$C_{10}H_{16}$
CAS-RN:	6004-38-2
Group No:	12-047

Experimental heat capacities (12.47.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1971BOY/SAN		372.0–390.0	2	n/a	99.9	melpt	p	BDHT	1973PER/COM
2003KON/TAN		351.0–358.2	4	0.20	99.9999	chrom	p	BSAO	1995TAN/SUN

Correlated heat capacities (12.47.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1971BOY/SAN	372.0–390.0	2	3.00	#	1.218	1.23	3.65	1.03	2
2003KON/TAN	351.0–358.2	4	0.20		0.977	5.73−2	0.20	−1.84−3	2

Parameters of regression polynomial (12.47.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	1.302	8.73−1	2.59	3.41−1	4

T/K	A_1	A_2	A_3	A_4	Uncert.
351.0–390.0	−2.425 46+1	1.511 08+1			IV

Deviation plot for Octahydro-4,7–methano-1H-indene (12–047) is given in Fig. 10.

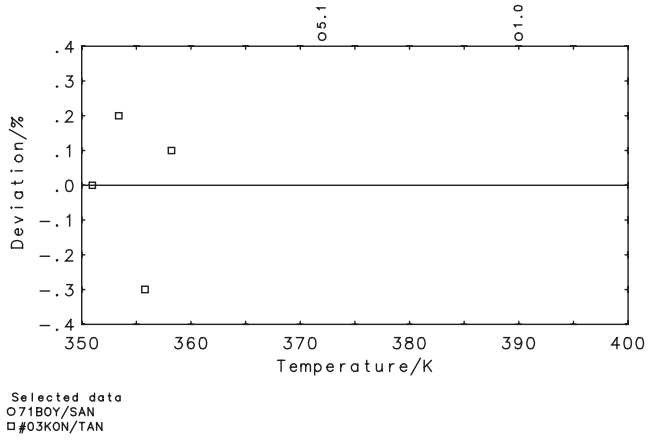

FIG. 10. Deviation plot for octahydro-4,7-methano-1*H*-indene (12-047).

6.2.2.5. 1,1′-bicyclopentyl (12-048)

Name:	1,1′-Bicyclopentyl
Formula:	$C_{10}H_{18}$
CAS-RN:	1636-39-1
Group No:	12-048

Experimental heat capacities (12.48.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1962GOL/BEL		310.9–422.0	3	n/a	98.9	chrom	p	BDHT	1963GUD/CAM
1963GUD/CAM	N	313.1–423.1	3	n/a	n/a	n/a	p	BDHT	1963GUD/CAM
1963GUD/CAM	N	313.1–423.1	3	n/a	n/a	n/a	p	BDHT	1963GUD/CAM
1976GOO/LEE		298.1	1	n/a	99.96	melpt	p	n/a	n/a
2004CHI/STE		235.7–388.8	20	0.10	99.98	melpt	sat	BSAO	1947HUF
2004CHI/STE		380.0–600.0	12	1.00	99.98	melpt	sat	BDHT	1989KNI/ARC

Reference	Notes
1963GUD/CAM	substance contained 0.01% cyclopentyl bromide
1963GUD/CAM	substance contained 0.10% cyclopentyl bromide

Correlated heat capacities (12.48.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1976GOO/LEE	298.1	1	2.00	#	0.042	2.40−2	0.08	2.40−2	1
2004CHI/STE	235.7–388.8	20	0.10		0.688	1.96−2	0.07	3.49−4	−3
2004CHI/STE	380.0–600.0	12	1.00		0.490	2.26−1	0.49	−5.58−2	−8

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1962GOL/BEL	(3.08, 9.95, −2.98, −3)	1963GUD/CAM	(3.05, 9.75, −2.93, −3)	
1963GUD/CAM	(3.14, 10.21, −3.09, −3)			

Parameters of regression polynomial (12.48.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	42	33	0.652	1.47−1	0.32	−1.93−2	−10
sat	42	33	0.593	1.16−1	0.26	−1.55−2	−8

T/K	A_1	A_2	A_3	A_4	Uncert.
235.7–600.0	2.668 52+1	−7.739 45	3.700 69	−2.942 12−1	III
235.7–600.0	2.727 40+1	−8.323 50	3.891 07	−3.146 12−1	III

Parameters of quasipolynomial equation (12.48.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	42	31	0.968	2.73−1	0.60	−5.97−2	−3

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
251.4–600.0	690.00	3.943 14+1	1.788 05	1.518 05+1	4.902 11+1	4.726 27+1	3.356 02+1	IV

Deviation plot for 1,1'-Bicyclopentyl (12–048) is given in Fig. 11.

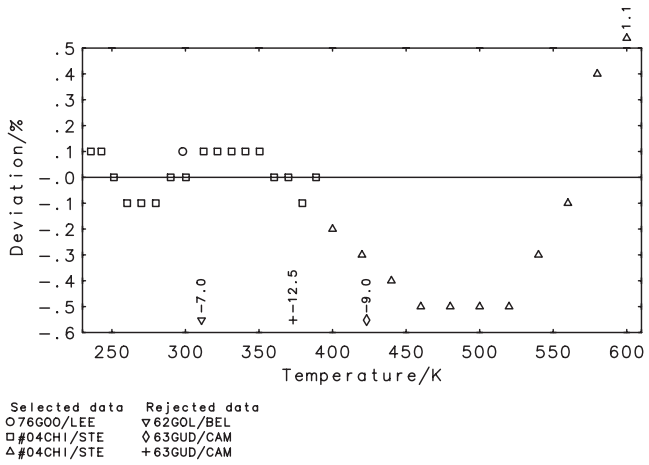

FIG. 11. Deviation plot for 1,1′-bicyclopentyl (12-048).

6.2.2.6. 1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane (12-063)

Name: 1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane

Formula: $C_{12}H_{20}$
CAS-RN: 702-79-4
Group No: 12-063

Experimental heat capacities (12.63.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1977STE/WAT	N	298.1	1		n/a	n/a	n/a	p	n/a	n/a
1996STE/CHI1		300.0–700.0	21	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2005VAR/DRU		251.3–359.0	78		0.30	99.973	melpt	p	BSAO	1997VAR/DRU1

Reference	Notes
1977STE/WAT	unspecified DSC calorimeter was used

Correlated heat capacities (12.63.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1996STE/CHI1	300.0–700.0	21	1.00	1.032	5.05−1	1.03	3.30−2	1
2005VAR/DRU	251.3–359.0	78	0.30	0.373	3.61−2	0.11	−4.71−4	6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1977STE/WAT	(1.17+1, 27.34, 1.17+1, 1)

Parameters of cubic spline polynomials (12.63.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	100	99	0.594	2.41−1	0.50	6.62−3	7
sat	100	99	0.547	1.92−1	0.44	8.14−3	9

T/K	A_1	A_2	A_3	A_4	Uncert.
251.3–650.0	7.185 37	7.506 63	1.959 70−1	−1.117 61−2	III
650.0–700.0	−6.691 32+4	3.089 38+4	−4.751 55+3	2.436 68+2	IV
251.3–650.0	8.681 38	6.149 08	5.986 55−1	−5.015 24−2	III
650.0–700.0	−4.081 33+4	1.884 71+4	−2.898 00+3	1.485 96+2	IV

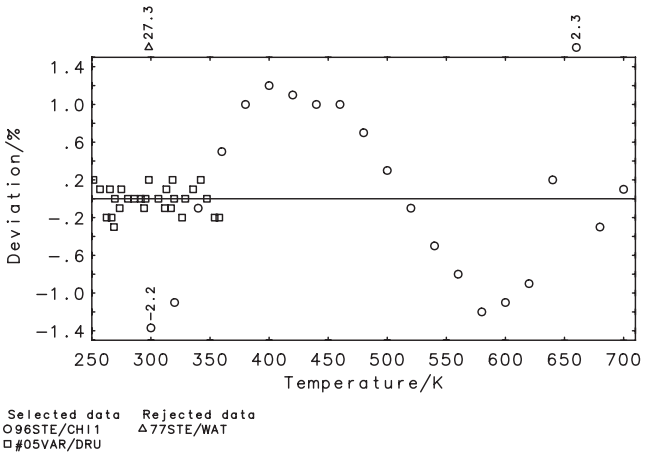

FIG. 12. Deviation plot for 1,3-dimethyltricyclo[3.3.1.1^{3,7}]decane (12-063).

Deviation plot for 1,3-Dimethyltricyclo[3.3.1.1^{3,7}]decane (12-063) is given in Fig. 12.

6.2.2.7. 1,1′-Bicyclohexyl (12-065)

Name:	1,1′-Bicyclohexyl
Formula:	$C_{12}H_{22}$
CAS-RN:	92-51-3
Group No:	12-065

Experimental heat capacities (12.65.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1957PIL		276.9	1		n/a	99.9985	melpt	*p*	BSAO	1957PIL
1962GOL/BEL		310.9–422.0	3	S	n/a	99.2	chrom	*p*	BDHT	1963GUD/CAM
1963GUD/CAM		313.1–483.1	4		n/a	99.2	chrom	*p*	BDHT	1963GUD/CAM
1983ORO/MRA		279.1–470.0	47	S	1.00	99.9	chrom	*p*	BDHT	1969PER/COM
1998CHI/COW		280.8–433.2	23		0.20	99.998	melpt	sat	BSAO	1988STE/ARC

6.2.2.8. 1,3,5-trimethyltricyclo[3.3.1.1^{3,7}]decane (12-071)

Name:	1,3,5-Trimethyltricyclo[3.3.1.1^{3,7}]decane
Formula:	$C_{13}H_{22}$
CAS-RN:	707-35-7
Group No:	12-071

Experimental heat capacities (12.71.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1977STE/WAT	N	298.1	1	n/a	99.95	melpt	*p*	n/a	n/a
2000DRU/VAR		258.0–356.8	86	0.20	99.98	melpt	*p*	BSAO	1997VAR/DRU1

Reference	Notes
1977STE/WAT	unspecified DSC calorimeter was used

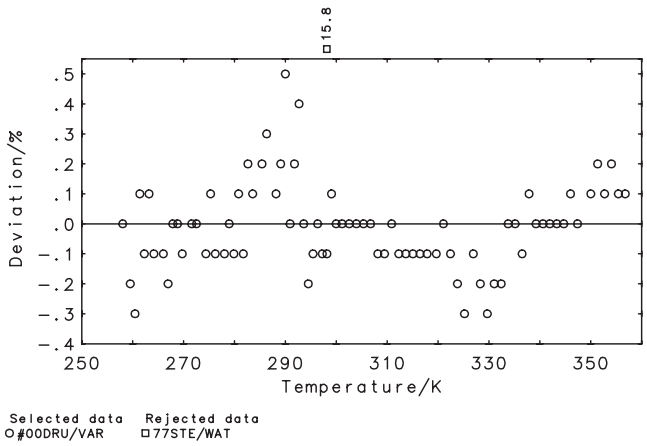

FIG. 13. Deviation plot for 1,3-trimethyltricyclo[3.3.1.1^{3,7}]decane (12-071).

Correlated heat capacities (12.71.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d/%	d_b/R	+/−
2000DRU/VAR	258.0–356.8	86	0.20	0.694	4.85–2	0.14	1.42−4	−7
Rejected data: Reference (d/R, d_r, d_b/R, +/−)								
1977STE/WAT	(6.50, 15.78, 6.50, 1)							

Parameters of regression polynomial (12.71.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	87	86	0.706	4.94−2	0.14	1.42−4	−7	
T/K		A_1		A_2		A_3	A_4	Uncert.
258.0−356.8		1.39565+1		4.46566		8.33593−1		III

Deviation plot for 1,3,5-Trimethyltricyclo[3.3.1.1^{3,7}] decane (12-071) is given in Fig. 13.

6.2.2.9. (3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene (12-126)

Name:	(3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene
Formula:	$C_{10}H_{16}$
CAS-RN:	2825-82-3
Group No:	12-126

Experimental heat capacities (12.126.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1978GOO/SCO		275.0–365.0	eqn	n/a	n/a	n/a	sat	BDHT	1969PER/COM
1978MOY/SAS		210.0–340.0	eqn	n/a	96.8	melpt	p	BDHT	1969PER/COM
1979SMI/GOO		298.1	1	n/a	n/a	n/a	p	BDHT	1969PER/COM
1980GOO/THO		260.0–465.0	eqn	n/a	99.98	chrom	sat	BDHT	1969PER/COM
2002CHI/HIL		193.1–273.1	10	n/a	99.8	melpt	p	BDHT	1995DIO/MAN

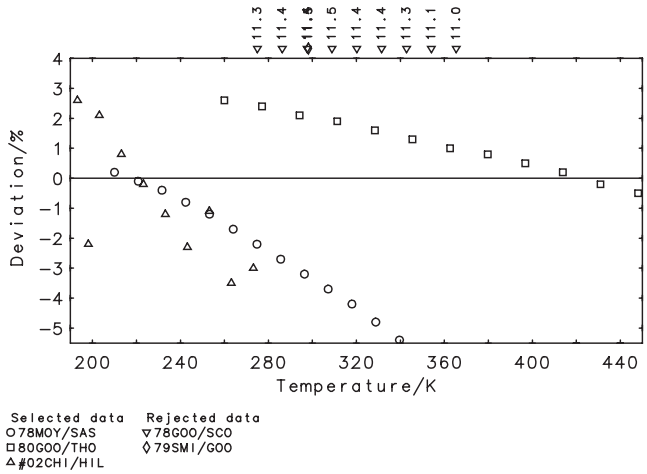

FIG. 14. Deviation plot for (3aα,4β,7β,7aα)-octahydro-4,7-methano-1*H*-indene (12-126).

Correlated heat capacities (12.126.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d/%	d_b/R	+/−
1978MOY/SAS	210.0–339.6	13	3.00	#	0.973	7.44−1	2.92	−5.76−1	−11
1980GOO/THO	260.0–465.2	13	1.50	#	0.969	3.82−1	1.45	2.52−1	7
2002CHI/HIL	193.1–273.1	10	2.00	#	1.075	4.44−1	2.15	−1.83−1	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1978GOO/SCO	(3.43, 11.31, 3.42, 9)	1979SMI/GOO	(3.26, 11.47, 3.26, 1)

Parameters of regression polynomial (12.126.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	46	36	1.046	5.79−1	2.37	−1.68−1	−8

T/K	A_1	A_2	A_3	A_4	Uncert.
193.1–465.2	7.415 54	4.507 48	4.876 04−1		IV

Deviation plot for (3aα,4β,7β,7aα)-Octahydro-4,7-methano-1*H*-indene (12-126) is given in Fig. 14.

6.2.2.10. Cyclodecane (12-138)

Name:	Cyclodecane
Formula:	$C_{10}H_{20}$
CAS-RN:	293-96-9
Group No:	12-138

Experimental heat capacities (12.138.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005HUA/SIM		288.0–319.0	eqn	n/a	99.0	error	p	BDHT	1999MO/YAN

Parameters of regression polynomial (12.138.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
288.0–318.9	5.643 62+1	−2.07691+1	4.321 14		V

6.2.2.11. 1-Ethyltricyclo[3.3.1.1^{3,7}]decane (12-139)

Name:	1-Ethyltricyclo[3.3.1.1^{3,7}]decane
Formula:	$C_{12}H_{20}$
CAS-RN:	770-69-4
Group No:	12-139

Experimental heat capacities (12.139.1)

Reference	Note	T/K	nPts	Err/%	Pur%	Method	Type	Calor.	Cal. Reference
2005VAR/DRU		228.2–373.9	109	0.30	99.93	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (12.139.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	109	109	0.386	3.80−2	0.12	7.95−5	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
228.2–373.9	1.377 30+1	3.389 19	8.080 97−1		II

6.2.2.12. Cyclododecane (12-140)

Name:	Cyclododecane
Formula:	$C_{12}H_{24}$
CAS-RN:	294-62-2
Group No:	12-140

Experimental heat capacities (12.140.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005HUA/SIM		335.0–368.0	eqn	n/a	99.0	error	p	BDHT	1999MO/YAN

Parameters of regression polynomial (12.140.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.000	3.82−6	0.00	−9.54−7	0

T/k	A_1	A_2	A_3	A_4	Uncert.
335.0–368.0	1.105 07+1	9.421 95	8.904 18−3		V

6.2.3. Sub group 13: unsaturated aliphatic hydrocarbons

6.2.3.1. 1-Nonyne (13-041)

Name:	1-Nonyne
Formula:	C_9H_{16}
CAS-RN:	3452-09-3
Group No:	13-041

Experimental heat capacities (13.41.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI4		290.0–450.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (13.41.3)

Type	nTot	nPts	$s_w s_w$	s/R	s_r/%	s_b/R	+/−
p	16	16	0.037	1.39−2	0.04	7.96−5	−1
T/K		A_1		A_2	A_3	A_4	Uncert.
290.0–450.5		1.407 41+1		6.038 58			III

Parameters of quasipolynomial equation (13.41.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	16	16	0.011	4.01−3	0.01	1.07−6	0

T/K	T/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
290.0–450.5	611.00	−2.255 41	4.645 28−2	1.38267+1	3.635 30+1	−4.618 43	1.973 82−1	III

6.2.4. Sub group 14: aromatic and unsaturated cyclic hydrocarbons

6.2.4.1. Benzene (14-003)

Name:	Benzene
Formula:	C_6H_6
CAS-RN:	71-43-2
Group No:	14-003

Experimental heat capacities (14.3.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1919DEJ		297.6–323.1	16		n/a	n/a	n/a	p	BSIO	1919DEJ
1921TRE		289.4–331.3	12		n/a	n/a	n/a	p	BSIO	1949WEI
1924WIL/DAN		305.0–335.0	eqn		n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1925WIL/DAN		293.1–333.1	5	S	n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1926AND/LYN		293.0–383.0	eqn		n/a	n/a	n/a	p	DSIO	1926AND/LYN
1930HUF/PAR1		281.1–300.0	6		1.00	n/a	n/a	p	BSIO	1925PAR
1931FIO/GIN	N	328.1–378.1	6	S	0.10	n/a	n/a	sat	BSIO	1931FIO/GIN
1933KOL/UDO	N	287.9	1		n/a	n/a	n/a	p	BSIT	1934KOL/UDO2
1937COH/BUI		283.1–295.1	7		n/a	n/a	n/a	p	BSAO	1920COH/MOE
1939PHI		301.4	1		n/a	n/a	n/a	p	BSIO	1949WEI
1941ZHD		281.4–318.8	3		n/a	n/a	n/a	p	BSIT	1934KOL/UDO2
1942ZIE/AND		283.5–322.6	9		2.00	99.99	melpt	p	BDHO	1937STU

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1947KUR		290.0–321.8	5		n/a	n/a	n/a	avg	DSIO	1947KUR
1948OLI/EAT		286.9–336.9	9		0.20	99.967	melpt	sat	BSAO	1943RUE/HUF
1948TSC1		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC5		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1951SIE/CRU	N	293.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1955STA/TUP		288.4–346.9	13		0.20	n/a	n/a	*p*	BSAO	1955STA/TUP
1956DUF/EVE	N	303.1–353.1	6	S	0.50	n/a	n/a	*p*	n/a	n/a
1960SWI/ZIE	N	316.3–322.1	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1962RAB/NIK		283.1–303.1	5	S	0.30	n/a	n/a	*p*	BSAO	1947SKU
1965FIN/GRU		300.0	1		0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1965KAU/BIT		293.1–349.1	8		1.00	n/a	n/a	*p*	FSIO	1965KAU/BIT
1967PAC		298.1	1		n/a	n/a	n/a	*p*	BDHT	1979DU/COM
1967RAS/GAN		293.1–353.1	4	S	0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1968REC1	N	298.0–313.0	eqn		n/a	n/a	n/a	*p*	BSAO	1968REC1
1971DES/BHA		298.1–318.1	3	S	1.00	n/a	n/a	*p*	BSIO	1958MUR/VAN
1971KHA/SUB	N	298.1–313.1	2		n/a	n/a	n/a	*p*	BSIO	1964MOE/THO
1974RAJ/SUB		298.1–323.1	3		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1975RAS/GRI	N	305.1–463.1	9		n/a	n/a	n/a	*p*	BDAO	1975RAS/GRI
1975SAN	N	433.1–493.1	6	S	1.00	n/a	n/a	*p*	FSIO	1975SAN
1976FOR/BEN2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1977BEL/BUB		298.1	1		n/a	n/a	n/a	*p*	BDCT	1968WAD
1977WIL/GRO		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1978GRO/WIL		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1981ATA/ELS		293.1	1		2.50	n/a	n/a	*p*	BDHO	1981ATA/ELS
1982GOR/SIM2		279.0–353.0	eqn		n/a	99.9	anal	*p*	FSIO	1983GOR/SIM
1982GRO/ING		298.1	1		n/a	98.5	melpt	*p*	FSIT	1971PIC/LED
1982TAN		293.1–303.1	3	S	0.30	99.99	melpt	*p*	FSIT	1971PIC/LED
1982WIL/FAR		298.1	1		n/a	98.5	melpt	*p*	FSIT	1971PIC/LED
1983GOR/SIM	N	283.8–348.5	12		0.25	99.9	anal	*p*	FSIO	1983GOR/SIM
1985OGA		298.1	1		0.10	n/a	n/a	*p*	FSIO	1985OGA
1985TAN		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986NAZ/BAS1		322.0–351.1	2		2.00	n/a	n/a	*p*	BDHO	1986NAZ/BAS1
1987GRO/ROU		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1987KAL/KOH		293.1–313.1	2		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1987TAN		293.1–303.1	3		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1988SHI/OGA1		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA
1989LAI/ROD		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1989PFE/SCH		313.1	1		n/a	n/a	n/a	*p*	BDCT	1968WAD
1989PRA/RAJ		318.1–333.1	4		3.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1990YAM/OGA		298.1	1		n/a	99.97	chrom	*p*	FSIO	1985OGA
1991CZA		298.5	1		2.00	n/a	n/a	*p*	BSIO	1979CZA
1991GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1991TAN/ADA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991WIL/JIM		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992MIY/TAM1		298.1	1		n/a	99.99	chrom	*p*	FSIO	1985OGA
1992MIY/TAM2		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA
1993DUR/AOU		303.0–347.0	23		n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1993GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994CHI/STE		300.0–540.0	13	S	1.00	99.9	chrom	sat	BDHT	1989KNI/ARC
1995DUR/AOU		303.0–347.0	eqn		2.00	99.99	anal	*p*	BDCT	1986MER/BEN
1995FUJ/TAM2		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA
1995NIS/OHO		298.1–308.1	2		n/a	99.95	chrom	*p*	FSIO	1985OGA

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997HU/TAM1		298.1	1	n/a	99.96	chrom	*p*	FSIO	1985OGA
1997TAN/NAK		298.1–303.1	2	n/a	100	chrom	*p*	FSIT	1971PIC/LED
1997TAN/TOY		298.1	1	0.15	99.95	chrom	*p*	FSIT	1971PIC/LED
1998WIL/EGG		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
2000TAK/TAM		298.1	1	n/a	99.99	chrom	*p*	FSIO	1985OGA
2002PAR/GON		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2003PAR/ZOU		288.1–348.1	13	0.30	99.5	anal	sat	BDCT	1983ROU/ROU
2006DIE/GME		295.1–350.1	12	3.00	99.9	chrom	*p*	BDHT	2004KIM/SHI

Reference	Notes
1931FIO/GIN	water content below 0.01%; data calculated using procedure by 1985WIL/CHA
1933KOL/UDO	same datum in 1934KOL/UDO2
1951SIE/CRU	heat of mixing calorimeter used
1956DUF/EVE	measured by a noncalorimetric method (piezothermometric)
1960SWI/ZIE	average values in the temperature ranges 294–339 K294–339 K and 294–350 K
1968REC1	same data in 1968REC2
1971KHA/SUB	reproducibility given as 0.3%
1975RAS/GRI	data above 343 K measured at superambient pressures up to 1.33 MPa
1975SAN	same data in 1976SAN/MEL; C_p at saturation curve extrapolated from high pressure measurements
1983GOR/SIM	same data in 1982GOR/GRI

6.2.4.2. Bicyclo[2.2.1]hepta-2,5-diene (14-009)

Name:	Bicyclo[2.2.1]hepta-2,5-diene
Formula:	C_7H_8
CAS-RN:	121-46-0
Group No:	14-009

Experimental heat capacities (14.9.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1973HAL/SMI		297.1	1	n/a	99.9	chrom	*p*	BDHT	1971DU/COM
1978STE	N	298.1	1	n/a	n/a	n/a	*p*	n/a	n/a
2004BYK/SMI		259.1–351.8	37	0.20	99.15	melpt	*p*	BSAO	1997VAR/DRU1

Reference	Notes
1978STE	unspecified DSC instrument used for measurement

Correlated heat capacities (14.9.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2004BYK/SMI	259.1–351.8	37	0.20	#	1.563	6.04−2	0.31	3.91−4	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1973HAL/SMI	(4.02, 28.80, −4.02, −1)	1978STE	(1.36, 7.01, 1.36, 1)

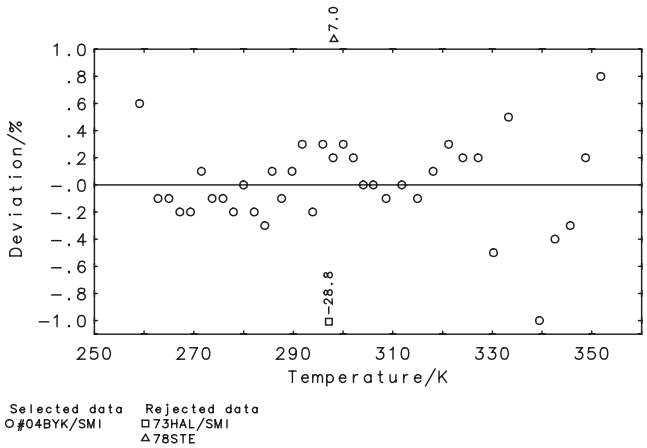

FIG. 15. Deviation plot for bicyclo[2.2.1]hepta-2,5-diene (14-009).

Parameters of regression polynomial (14.9.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	39	37	1.655	6.40−2	0.33	3.91−4	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
259.1–351.8	−5.600 36+1	6.709 22+1	−2.148 98+1	2.453 53	IV

Deviation plot for Bicyclo[2.2.1]hepta-2,5-diene (14-009) is given in Fig. 15.

6.2.4.3. Methylbenzene (14-011)

Name:	Methylbenzene
Formula:	C_7H_8
CAS-RN:	108-88-3
Group No:	14-011

Experimental heat capacities (14.11.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		304.8–341.3	7	S	n/a	n/a	n/a	avg	DSIO	1881VON
1886SCH		309.3–329.0	11	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1907BAT	N	181.1–248.1	6		n/a	n/a	n/a	p	BSIO	1907BAT
1924WIL/DAN		305.0–348.0	eqn		n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1925WIL/DAN		293.1–333.1	5	S	n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1929KEL5	N	183.8–284.4	11		n/a	n/a	n/a	p	BSIO	1929KEL1
1930SOU/AND	N	183.8–244.8	7		0.50	n/a	n/a	p	BSAO	1930SOU/AND
1931SMI/AND1		184.4–298.5	9		n/a	n/a	n/a	p	DSIO	1926AND/LYN
1935AOY/KAN		195.2–227.8	2		n/a	n/a	n/a	p	BSAO	1935AOY/KAN
1937VOL		298.1	1		n/a	n/a	n/a	p	BSIO	1937VOL
1941ZHD		278.5–320.4	3		n/a	n/a	n/a	p	BSIT	1934KOL/UDO2
1947KUR		241.9–310.5	4		n/a	n/a	n/a	avg	DSIO	1947KUR
1948TSC1		295.1	1		n/a	n/a	n/a	p	BSIO	1948TSC1
1948TSC5		295.1	1		n/a	n/a	n/a	p	BSIO	1948TSC1
1956SCH/GOT		270.0–292.5	10		2.00	n/a	n/a	p	BSAO	1933SOU/BRI
1958SWI/ZIE2	N	323.9–333.2	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1962SCO/GUT		183.2–371.0	23		0.20	99.999	melpt	sat	BSAO	1947HUF

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1966HWA/ZIE		180.9–304.4	34		n/a	99.99	melpt	*p*	BSAO	1945SCO/MEY
1967RAS/GAN		293.1–373.1	5	S	0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1971DES/BHA		298.1–318.1	3	S	1.00	n/a	n/a	*p*	BSIO	1958MUR/VAN
1973AKH/EKS		298.1	1		0.20	n/a	n/a	*p*	FSIO	1959RIB/EGO
1974RAJ/SUB		298.1–323.1	3		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1975HOL/ZIE		162.0–312.0	eqn		0.20	n/a	n/a	*p*	BSAO	1945SCO/MEY
1975PED/KAY		300.6–347.3	19		n/a	n/a	n/a	*p*	BSIO	1975PED/KAY
1975RAS/GRI	N	303.0–462.7	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1976FOR/BEN1		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1976SAN/MEL	N	393.1–503.1	8	S	1.00	n/a	n/a	*p*	FSIO	1975SAN
1977BEL/BUB		298.1	1		n/a	n/a	n/a	*p*	BDCT	1968WAD
1977FOR/BEN		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1977WIL/GRO		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1979AND/GRI	N	293.1–373.3	9		0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1980NEF/FIL		300.0–520.0	12	S	n/a	n/a	n/a	sat	BDHO	1984FIL/LAU
1981ATA/ELS		293.1	1		2.50	n/a	n/a	*p*	BDHO	1981ATA/ELS
1982GRO/ING		298.1	1		0.30	99.5	estim	*p*	FSIT	1971PIC/LED
1982WIL/FAR		298.1	1		0.30	99.5	estim	*p*	FSIT	1971PIC/LED
1984STE/OLS		266.1–318.1	11	S	n/a	99.5	melpt	*p*	BDHT	1969PER/COM
1985COS/PAT6		298.2	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1986ROU/GRO		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1987OKH/RAZ		181.4–380.4	15		0.30	n/a	n/a	sat	BDAO	1987OKH/RAZ
1988SHI/OGA1		298.1	1		n/a	99.9	Chrom	*p*	FSIO	1985OGA
1988STE/CHI		300.0–580.0	29	S	n/a	n/a	n/a	sat	BDHT	1989KNI/ARC
1989PRA/RAJ		318.1–333.1	4		3.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1990RAO/RAJ		318.1–333.1	4		4.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1991COB/GAR		298.1–368.1	4		n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
1991TAN/ADA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991WIL/JIM		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1993CON/GIR1		298.0–359.0	eqn		5.00	n/a	n/a	sat	BDHT	1993CON/GIR1
1993GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994CHI/STE		300.0–570.0	15	S	1.00	99.9	chrom	sat	BDHT	1989KNI/ARC
1994GRO/ROU		298.1	1		n/a	99.0	chrom	*p*	FSIT	1971PIC/LED
1994JIM/ROM		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994PRA/RAJ		293.1–323.1	4		n/a	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1995FUJ/TAM2		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA
1997TAN/NAK		298.1–303.1	2		n/a	100	chrom	*p*	FSIT	1971PIC/LED
1997TAN/TOY		298.1	1		0.15	99.95	chrom	*p*	FSIT	1971PIC/LED
1998WIL/EGG		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1999BRO/CAL1		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
2000BEC/AUF	N	302.0–337.0	8		0.30	99.95	chrom	sat	BDCT	2000BEC/AUF
2000BEC/AUF	N	288.1–353.2	14		0.20	99.95	chrom	sat	BDCT	2000BEC/AUF
2001BEC/GME		310.0–370.0	13		0.50	99.95	chrom	sat	BDCT	2000BEC/AUF
2002CER/TOV		278.1–335.6	24		n/a	99.8	chrom	*p*	BDHT	1969PER/COM
2002PAR/ZOU		278.1–348.1	15		n/a	99.5	chrom	sat	BDCT	1983ROU/ROU
2003PAR/ZOU		288.1–348.1	13		0.30	99.5	anal	sat	BDCT	1983ROU/ROU

Reference	Notes
1907BAT	same data in 1908BAT
1929KEL5	high sample purity
1930SOU/AND	high sample purity
1958SWI/ZIE2	average values in the temperature ranges 294–354 and 294–372 K

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1975RAS/GRI	data above 364 K measured at superambient pressures up to 0.72 MPa								
1976SAN/MEL	C_p at saturation curve extrapolated from high pressure measurements								
1979AND/GRI	grade: pure								
2000BEC/AUF	"step by step" method was used								
2000BEC/AUF	"three-step" method was used								

6.2.4.4. Ethynylbenzene (14-015)

Name:	Ethynylbenzene
Formula:	C_8H_6
CAS-RN:	536-74-3
Group No:	14-015

Experimental heat capacities (14.15.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931SMI/AND1		231.7–298.5	6		n/a	99.0	estim	*p*	DSIO	1926AND/LYN
1982LEB/BYK		228.0–330.0	4	S	0.30	98.4	melpt	*p*	BSAO	1976LEB/LIT
2002STE/CHI3		303.0–393.0	eqn		1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (14.15.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1931SMI/AND1	231.7–298.5	6	1.20	#	0.464	1.14−1	0.56	−9.81−2	−6
1982LEB/BYK	228.0–330.0	4	1.00	#	0.666	1.42−1	0.67	2.65−2	2
2002STE/CHI3	303.0–393.4	9	1.00		0.308	6.93−2	0.31	3.54−2	1

Parameters of regression polynomial (14.15.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.511	1.16−1	0.55	−8.60−3	−3
sat	19	19	0.511	1.16−1	0.55	−8.60−3	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
228.0–393.4	4.508 51+1	−2.858 46+1	9.898 03	−9.907 77−1	III
228.0–393.4	4.508 51+1	−2.858 46+1	9.898 03	−9.907 77−1	III

Parameters of quasipolynomial equation (14.15.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	19	19	0.534	1.21−1	0.57	−2.38−3	−2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
228.0–393.4	650.00	1.351 65+3	1.478 89+2	−1.338 76+2	1.273 61+3	1.968 95+2	8.933 81+2	III

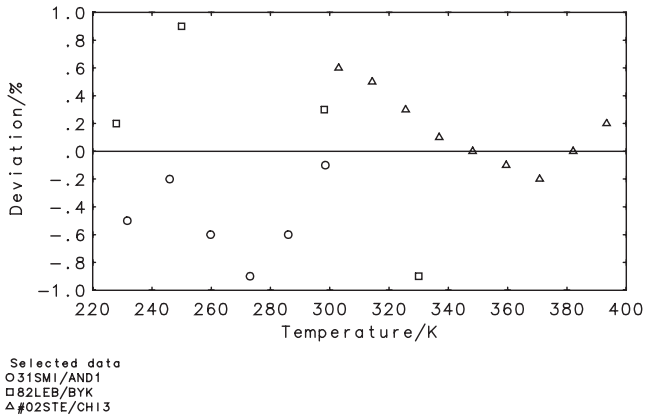

FIG. 16. Deviation plot for ethynylbenzene (14-015).

Deviation plot for Ethynylbenzene (14-015) is given in Fig. 16.

6.2.4.5. 1,3-Dimethylbenzene (14-019)

Name:	1,3-Dimethylbenzene
Formula:	C_8H_{10}
CAS-RN:	108-38-3
Group No:	14-019

Experimental heat capacities (14.19.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		308.9–334.8	11	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1924WIL/DAN		303.0–348.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1930HUF/PAR1	N	217.0–275.3	6		1.00	n/a	n/a	*p*	BSIO	1925PAR
1943PIT/SCO	N	231.4–318.2	11		0.20	97.66	melpt	*p*	BSIO	1928LAT/GRE
1947KUR		309.8–347.7	3		n/a	n/a	n/a	avg	DSIO	1947KUR
1948TSC3		293.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC6		294.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1958SWI/ZIE2	N	336.8	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1975RAS/GRI	N	302.9–462.5	9		1.00	n/a	n/a	*p*	BDAO	1975RAS/GRI
1975SAN	N	411.1–540.2	8	S	1.00	n/a	n/a	*p*	FSIO	1975SAN
1977FOR/BEN		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1979FOR/BEN		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1991TAN/ADA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1992JAI/CHA		303.6–321.6	7		n/a	98.	anal	*p*	BDCT	1991BAN/GAR
1993GAR/BAN		318.1–373.1	12		n/a	99.3	chrom	*p*	BDCT	1991BAN/GAR
1993GRO/ROU		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED
1997CHI/KNI4		232.3–423.4	17		0.10	99.9	melpt	sat	BSAO	1988STE/ARC
1997CHI/KNI4		440.0–550.0	7	S	1.00	99.9	melpt	sat	BDHT	1989KNI/ARC
2003PAR/ZOU		288.1–348.1	13		0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8		0.50	99.0	anal	sat	BDCT	1991BAN/GAR

Reference	Notes
1930HUF/PAR1	low sample purity
1943PIT/SCO	corrected for content of 1,4-dimethylbenzene
1958SWI/ZIE2	average value in the temperature range 333–373 K
1975RAS/GRI	data above 384 K measured at superambient pressures up to 0.45 MPa
1975SAN	same data in 1976SAN/MEL; C_p at saturation line extrapolated from high pressure measurement

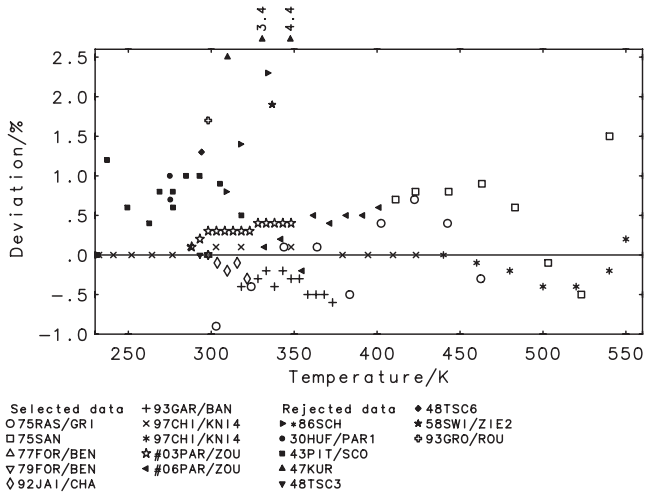

FIG. 17. Deviation plot for 1,3-dimethylbenzene (14-019).

Correlated heat capacities (14.19.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1975RAS/GRI	303.0–462.5	9	1.00		0.488	1.22−1	0.49	−7.48−3	1
1975SAN	411.1–540.2	8	1.00		0.838	2.68−1	0.84	1.84−1	4
1977FOR/BEN	298.1	1	0.50	#	0.003	3.78−4	0.00	3.78−4	0
1979FOR/BEN	298.1	1	0.30		0.131	8.56−3	0.04	8.56−3	1
1992JAI/CHA	303.6–321.6	7	0.50	#	0.315	3.56−2	0.16	−3.18−2	−7
1993GAR/BAN	318.1–373.1	12	0.50	#	0.799	9.63−2	0.40	−9.10−2	−12
1997CHI/KNI4	232.3–423.4	17	0.30	#	0.224	1.52−2	0.07	1.02−2	9
1997CHI/KNI4	440.0–550.0	7	0.50	#	0.495	8.16−2	0.25	−4.52−2	−5
2003PAR/ZOU	288.1–348.1	13	0.70	#	0.453	7.32−2	0.32	7.01−2	13
2006PAR/ZOU	332.2–401.3	8	0.70	#	0.586	1.05−1	0.41	8.36−2	6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1886SCH	(4.09−1, 1.74, 3.86−1, 11)	1924WIL/DAN	(6.06−1, 2.71, −6.06−1, −8)
1930HUF/PAR1	(1.88−1, 0.89, 1.85−1, 2)	1943PIT/SCO	(1.77−1, 0.83, 1.70−1, 10)
1947KUR	(8.54−1, 3.50, 8.26−1, 3)	1948TSC3	(9.13−3, 0.04, 9.13−3, 1)
1948TSC6	(2.90−1, 1.32, 2.90−1, 1)	1958SWI/ZIE2	(4.63−1, 1.93, 4.63−1, 1)
1991TAN/ADA	(1.67−2, 0.08, −1.67−2, −1)	1993GRO/ROU	(3.79−1, 1.71, 3.79−1, 1)

Parameters of cubic spline polynomials (14.19.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	127	83	0.556	1.16−1	0.41	1.86−2	10
sat	127	83	0.543	1.13−1	0.40	1.90−2	8

T/K	A_1	A_2	A_3	A_4	Uncert.
232.3–400.0	2.139 40+1	−5.428 19	2.442 23	−1.921 57−1	II
400.0–550.0	−2.304 50+1	2.790 11+1	−5.890 08	5.022 02−1	IV
232.3–400.0	2.124 39+1	−5.308 08	2.414 11	−1.905 16−1	II
400.0–550.0	−1.067 23+1	1.862 91+1	−3.570 17	3.081 74−1	IV

Parameters of quasipolynomial equation (14.19.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	127	83	0.886	1.23−1	0.46	4.55−3	6

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
232.3–550.0	617.05	−2.420 55	4.710 75−2	1.216 01+1	1.294 26+1	6.926 29	1.162 71	III

Deviation plot for 1,3–Dimethylbenzene (14-019) is given in Fig. 17.

6.2.4.6. 1,4-Dimethylbenzene (14-020)

Name:	1,4-Dimethylbenzene
Formula:	C_8H_{10}
CAS-RN:	106-42-3
Group No:	14-020

Experimental heat capacities (14.20.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		312.2–335.7	6	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1924WIL/DAN		303.0–348.0	eqn		n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1930HUF/PAR1		290.7–299.4	5		1.00	n/a	n/a	p	BSIO	1925PAR
1943PIT/SCO		292.0–354.6	10		0.20	99.98	melpt	p	BSIO	1928LAT/GRE
1947COR/GIN		293.1–573.2	15	S	0.20	99.9	melpt	sat	DSTO	1950GIN/DOU
1947KUR		309.3–349.1	3		n/a	n/a	n/a	avg	DSIO	1947KUR
1948TSC3		293.1	1		n/a	n/a	n/a	p	BSIO	1948TSC1
1948TSC6		294.1	1		n/a	n/a	n/a	p	BSIO	1948TSC1
1958SWI/ZIE2	N	336.6–347.0	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1961ROU		298.0–315.9	20		n/a	n/a	n/a	p	BSAO	1961ROU
1971KHA/SUB	N	298.1–313.1	2		n/a	n/a	n/a	p	BSIO	1964MOE/THO
1975RAS/GRI	N	303.6–462.9	9		1.00	n/a	n/a	p	BDAO	1975RAS/GRI
1977BEL/BUB		298.1	1		n/a	n/a	n/a	p	BDCT	1968WAD
1977FOR/BEN		298.1	1		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1977WIL/GRO		298.1	1		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1979FOR/BEN		298.1	1		0.30	n/a	n/a	p	FSIT	1971PIC/LED
1979OTT/GOA		288.1–328.1	9	S	0.30	99.9	melpt	p	FSIT	1971PIC/LED
1985COS/PAT7		298.2	1		n/a	99.	anal	p	FSIT	1971PIC/LED
1988MES/FIN		295.4–373.4	11		0.10	99.996	melpt	sat	BSAO	1947HUF
1989PFE/SCH	N	313.1	1		n/a	n/a	n/a	p	BDCT	1968WAD
1989PRA/RAJ		318.1–333.1	4		3.00	n/a	n/a	p	BDHT	1989PRA/RAJ
1991TAN/ADA		298.1	1		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1991WIL/JIM		298.1	1		n/a	99.	anal	p	FSIT	1971PIC/LED
1992JAI/CHA		303.6–321.6	7		n/a	98.	anal	p	BDCT	1991BAN/GAR
1993GAR/BAN		318.1–373.1	12		n/a	99.7	chrom	p	BDCT	1991BAN/GAR
1997CHI/KNI2		380.0–550.0	10	S	1.00	99.996	melpt	sat	BDHT	1989KNI/ARC
2005VAL/TRO		288.1–308.1	3		n/a	99.0	chrom	p	BDHT	1969PER/COM

Reference	Notes
1958SWI/ZIE2	average values in the temperature ranges 294–379 and 295−399 K
1971KHA/SUB	reproducibility given as 0.3%
1975RAS/GRI	Data above 386 K measured at superambient pressures up to 0.49 MPa
1989PFE/SCH	the publish value at 298.15 K the same as 1977BEL/BUB

Correlated heat capacities (14.20.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1947COR/GIN	293.1–573.2	15	2.00	#	0.372	2.29−1	0.74	−9.70−2	−11
1975RAS/GRI	303.6–462.9	9	1.00		0.425	1.02−1	0.42	−6.17−2	−5
1977FOR/BEN	298.1	1	0.50	#	0.335	3.66−2	0.17	−3.66−2	−1
1979FOR/BEN	298.1	1	0.30		0.296	1.94−2	0.09	−1.94−2	−1
1979OTT/GOA	288.1–328.1	9	0.30		0.873	5.75−2	0.26	−3.35−2	−7
1988MES/FIN	295.4–373.4	11	0.10		0.486	1.10−2	0.05	7.30−3	6
1989PFE/SCH	313.1	1	0.50	#	0.481	5.43−2	0.24	5.43−2	1
1991TAN/ADA	298.1	1	0.50	#	0.438	4.79−2	0.22	−4.79−2	−1
1991WIL/JIM	298.1	1	0.50	#	0.287	3.15−2	0.14	3.15−2	1
1992JAI/CHA	303.6–321.6	7	0.30	#	0.731	4.92−2	0.22	−4.77−2	−7
1997CHI/KNI2	380.0–550.0	10	1.00		0.278	8.91−2	0.28	1.19−2	0
2005VAL/TRO	288.1–308.1	3	1.00	#	0.234	5.18−2	0.23	4.72−2	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1886SCH	(2.54−1, 1.08, 2.40−1, 6)	1924WIL/DAN	(7.45−1, 3.37, −7.41−1, −8)
1930HUF/PAR1	(2.21−1, 1.02, −2.15−1, −5)	1943PIT/SCO	(4.40−1, 1.87, 1.55−1, 6)
1947KUR	(8.48−1, 3.46, 8.07−1, 3)	1948TSC3	(3.26−1, 1.52, −3.26−1, −1)
1948TSC6	(3.13−1, 1.46, −3.13−1, −1)	1958SWI/ZIE2	(2.89−1, 1.20, 2.88−1, 2)
1961ROU	(8.06−1, 3.49, 8.02−1, 20)	1971KHA/SUB	(1.04−1, 0.47, −9.36−2, −2)
1977BEL/BUB	(3.35−1, 1.55, −3.35−1, −1)	1977WIL/GRO	(6.59−2, 0.30, −6.59−2, −1)
1985COS/PAT7	(1.85−1, 0.84, 1.85−1, 1)	1989PRA/RAJ	(3.05−1, 1.29, 2.80−1, 4)
1993GAR/BAN	(1.75−1, 0.73, −1.73−1, −12)		

Parameters of cubic spline polynomials (14.20.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	146	69	0.538	1.26−1	0.43	−3.37−2	−22
sat	146	69	0.527	1.09−1	0.40	−3.78−2	−20

T/K	A_1	A_2	A_3	A_4	Uncert.
288.1–420.0	1.891 82+1	−3.528 33	1.987 19	−1.570 30−1	II
420.0–573.2	−5.117 13+1	4.653 56+1	−9.932 80	7.890 00−1	IV
288.1–420.0	1.867 71+1	−3.382 53	1.966 82	−1.575 19−1	II
420.0–573.2	−2.816 55+1	3.007 65+1	−5.999 61	4.747 37−1	IV

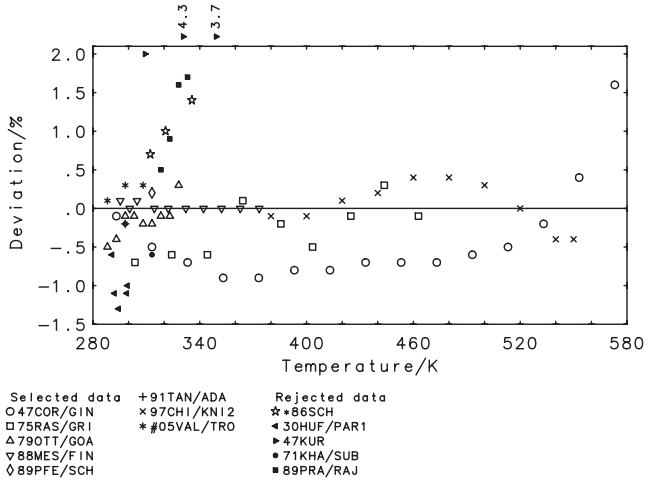

FIG. 18. Deviation plot for 1,4-dimethylbenzene (14-020).

Deviation plot for 1,4–Dimethylbenzene (14-020) is given in Fig. 18.

6.2.4.7. Ethylbenzene (14-021)

Name:	Ethylbenzene
Formula:	C_8H_{10}
CAS-RN:	100-41-4
Group No:	14-021

Experimental heat capacities (14.21.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		304.8–362.1	8	S	n/a	n/a	n/a	avg	DSIO	1881VON
1886SCH		309.0–335.7	11	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1924WIL/DAN		303.0–343.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1930HUF/PAR1		185.0–304.9	16		1.00	n/a	n/a	*p*	BSIO	1925PAR
1931BLA/LEI		286.1–368.1	25		3.00	n/a	n/a	sat	BSIO	1931BLA/LEI
1931SMI/AND1		184.4–298.5	9		n/a	99.9	estim	*p*	DSIO	1926AND/LYN
1934KOL/UDO2	N	302.7	1		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1944GUT/SPI		181.5–305.4	16		0.10	99.93	melpt	*p*	BSAO	1943RUE/HUF
1945SCO/BRI		178.2–300.0	27	S	0.10	99.993	melpt	sat	BSAO	1933SOU/BRI
1947KUR		308.8–372.8	4		n/a	n/a	n/a	avg	DSIO	1947KUR
1948TSC1		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC5		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1976FOR/BEN2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1977FOR/BEN		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1979AND/GRI	N	293.3–393.0	10		0.50	n/a	n/a	sat	BSAO	1967RAS/GAN
1979FOR/BEN		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1983GRO/FAR1		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991TAN/ADA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991WIL/JIM		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1992JAI/CHA		303.6–321.6	7		n/a	98.	anal	*p*	BDCT	1991BAN/GAR
1993GAR/BAN		318.1–373.1	12		n/a	99.5	chrom	*p*	BDCT	1991BAN/GAR
1995FUJ/TAM1		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA
1997CHI/KNI3		183.4–412.4	18		0.10	99.99	melpt	sat	BSAO	1988STE/ARC
1997CHI/KNI3		420.0–550.0	8	S	1.00	99.99	melpt	sat	BDHT	1989KNI/ARC
2003PAR/ZOU		288.1–348.1	13		0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–391.4	7		0.50	99.0	anal	sat	BDCT	1991BAN/GAR

Reference	Notes
1934KOL/UDO2	same datum in 1934KOL/UDO1
1979AND/GRI	error 0.5% below 373 K and 0.8% at 433 K

Correlated heat capacities (14.21.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1944GUT/SPI	181.5–305.4	16	0.50	#	0.118	1.18−2	0.06	5.26−3	7
1945SCO/BRI	178.1–300.0	27	0.50	#	0.181	1.85−2	0.09	1.78−2	27
1976FOR/BEN2	298.1	1	0.30		0.147	9.88−3	0.04	−9.88−3	−1
1977FOR/BEN	298.1	1	0.50	#	0.327	3.65−2	0.16	−3.65−2	−1
1979AND/GRI	293.3–393.0	10	0.50		1.107	1.41−1	0.55	−1.00−1	−6
1979FOR/BEN	298.1	1	0.50	#	0.313	3.49−2	0.16	−3.49−2	−1
1983GRO/FAR1	298.1	1	0.50	#	0.110	1.23−2	0.05	−1.23−2	−1
1991TAN/ADA	298.1	1	0.50	#	0.282	3.15−2	0.14	−3.15−2	−1

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1991WIL/JIM	298.1	1	0.50	#	0.078	8.67−3	0.04	−8.67−3	−1
1992JAI/CHA	303.6–321.6	7	1.00	#	0.236	5.45−2	0.24	5.11−2	7
1997CHI/KNI3	183.4–412.4	18	0.10		0.344	8.19−3	0.03	5.58−4	−1
1997CHI/KNI3	420.0–550.0	8	1.00		0.455	1.54−1	0.45	−2.22−2	−4
2003PAR/ZOU	288.1–348.1	13	0.30		0.521	3.61−2	0.16	2.59−3	1
2006PAR/ZOU	332.2–391.4	7	1.00	#	0.590	1.52−1	0.59	1.32−1	5

Rejected data: Reference d/R, d_r, d_b/R, (+/−)

1881VON	(3.44−1, 1.42, −4.39−2, 0)	1886SCH	(3.27−1, 1.37, 3.12−1, 11)
1924WIL/DAN	(6.31−1, 2.79, −6.27−1, −4)	1930HUF/PAR1	(2.92−1, 1.36, −2.45−1, −16)
1931BLA/LEI	(8.69−1, 3.42, 4.37−1, 15)	1931SMI/AND1	(4.38−1, 2.27, −4.11−1, −9)
1934KOL/UDO2	(1.04, 4.82, −1.04, −1)	1947KUR	(7.75−1, 2.98, 6.72−1, 4)
1948TSC1	(4.57−2, 0.20, 4.57−2, 1)	1948TSC5	(1.53−1, 0.68, 1.53−1, 1)
1993GAR/BAN	(1.55−1, 0.65, −1.44−1, −12)	1995FUJ/TAM1	(1.46−1, 0.66, −1.46−1, −1)

Parameters of cubic spline polynomials (14.21.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	205	112	0.472	7.50−2	0.28	5.15−3	30
sat	205	112	0.459	6.76−2	0.26	5.85−3	31

T/K	A_1	A_2	A_3	A_4	Uncert.
178.2–320.0	2.451 11+	−8.616 48	3.690 08	−3.497 39−1	I
320.0–550.0	1.151 69+1	3.565 56	−1.168 10−1	4.681 17−2	III
178.2–320.0	2.440 43+	−8.486 37	3.638 52	−3.430 91−1	I
320.0–550.0	1.358 82+1	1.653 77	4.697 30−1	−1.300 88−2	IV

Parameters of quasipolynomial equation (14.21.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	209	112	1.962	1.32−1	0.53	−3.36−2	−40

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
178.1–550.0	617.24	4.482 04	7.067 87−2	1.583 52+1	9.530 94	1.492 07+1	1.160 73+1	V

Deviation plot for Ethylbenzene (14-021) is given in Fig. 19.

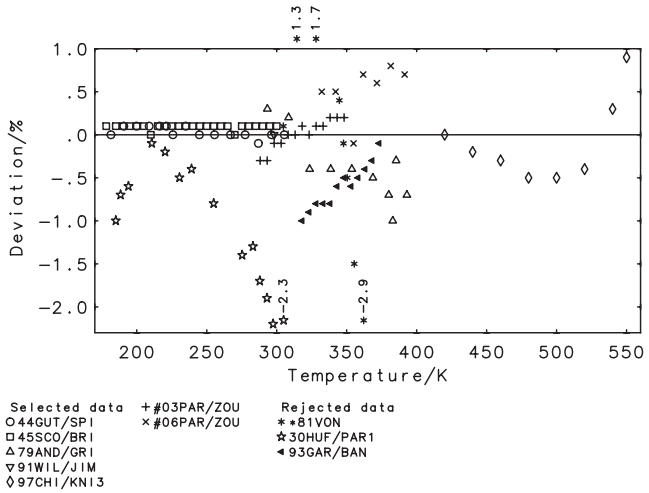

FIG. 19. Deviation plot of for ethylbenzene (14-021).

6.2.4.8. (1-Methylethyl)benzene (14-028)

Name:	(1-Methylethyl)benzene
Formula:	C_9H_{12}
CAS-RN:	98-82-8
Group No:	14-028

Experimental heat capacities (14.28.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1934KOL/UDO2	N	302.0	1		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1947KUR		308.8–359.6	4		n/a	n/a	n/a	avg	DSIO	1947KUR
1952SCH/SAG		299.8–366.5	13	S	1.00	99.8	estim	*p*	BSAO	1939SAG/EVA
1973KIS/SUG		179.9–313.1	45		n/a	99.93	melpt	sat	BSAO	1965SUG/SEK
1979AND/GRI	N	296.0–412.8	7		0.50	n/a	n/a	sat	BSAO	1967RAS/GAN
1995FUJ/TAM1		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA
2003PAR/ZOU		288.1–328.1	9		0.30	98.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8		1.00	98.0	anal	sat	BDCT	1991BAN/GAR

Reference	Notes
1934KOL/UDO2	same datum in 1934KOL/UDO1
1979AND/GRI	error 0.5% below 373 K and 0.8% at 433 K

Correlated heat capacities (14.28.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1973KIS/SUG	179.9–313.1	45	0.50	#	0.158	1.99−2	0.08	6.21−3	8
1979AND/GRI	296.0–412.8	7	0.50		0.747	1.06−1	0.37	−8.36−2	−3
2003PAR/ZOU	288.1–328.1	9	0.30		0.398	3.12−2	0.12	−1.12−5	1
2006PAR/ZOU	332.2–401.3	8	1.00		0.576	1.72−1	0.58	1.59−1	8

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1934KOL/UDO2	(2.13, 8.91, −2.13, −1)	1947KUR	(1.47−1, 0.54, −6.95−2, −2)
1952SCH/SAG	(4.85−1, 1.88, −3.81−1, −9)	1995FUJ/TAM1	(1.95, 8.15, −1.95, −1)

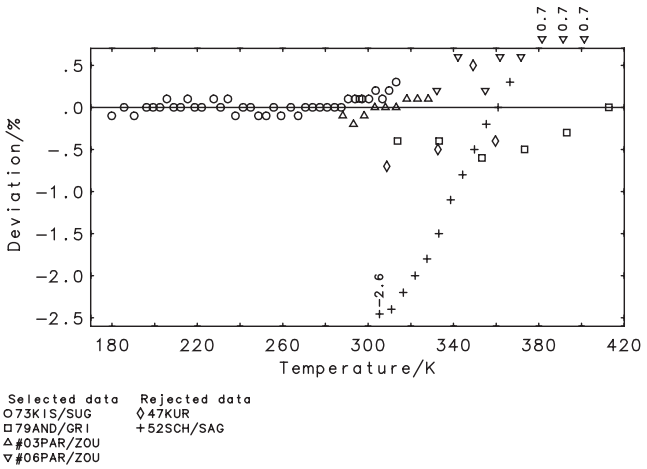

FIG. 20. Deviation plot for (1-methylethyl)benzene (14-028).

Parameters of cubic spline polynomials (14.28.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	88	69	0.377	7.32−2	0.25	1.40−2	14

T/K	A_1	A_2	A_3	A_4	Uncert.
179.9–300.0	2.723 41+1	−9.488 84	4.336 58	−4.384 37−1	II
300.0–412.8	1.834 51+1	−5.999 14−1	1.373 60	−1.092 18−1	IV

Parameters of quasipolynomial equation (14.28.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	88	69	0.433	7.41−2	0.26	1.29−2	7

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
179.9–412.8	631.10	1.524 31+2	1.246 64+1	7.549 88	1.399 92+2	6.613 56+1	1.066 72+2	III

Deviation plot for (1–Methylethyl)benzene (14-028) is given in Fig. 20.

6.2.4.9. Propylbenzene (14-029)

Name:	Propylbenzene
Formula:	C_9H_{12}
CAS-RN:	103-65-1
Group No:	14-029

Experimental heat capacities (14.29.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		308.6–346.9	9	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1948TSC1		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC5		294.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1965MES/TOD2		180.9–370.5	23		0.10	99.97	melpt	sat	BSAO	1947HUF
1983GRO/FAR2		298.1	1		n/a	99.0	estim	*p*	FSIT	1971PIC/LED
1995FUJ/TAM1		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA
2003PAR/ZOU		288.1–348.1	13		0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–391.4	7		0.50	99.0	anal	sat	BDCT	1991BAN/GAR

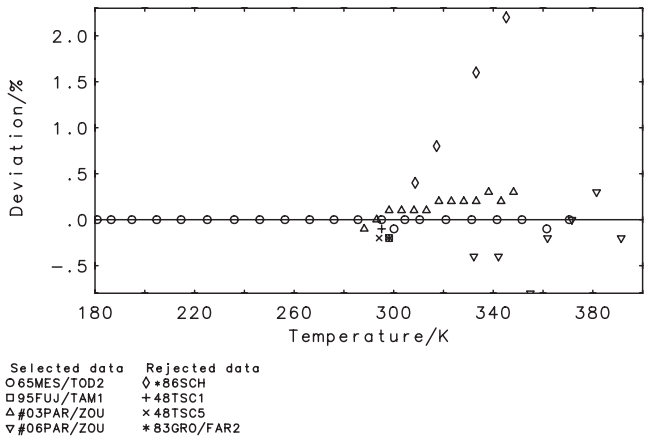

FIG. 21. Deviation plot for propylbenzene (14-029).

Correlated heat capacities (14.29.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1965MES/TOD2	180.9–370.5	23	0.10		0.261	6.87−3	0.03	−1.97−3	−3
1995FUJ/TAM1	298.1	1	0.50	#	0.474	6.10−2	0.24	−6.10−2	−1
2003PAR/ZOU	288.1–348.1	13	0.30		0.571	4.73−2	0.17	3.68−2	9
2006PAR/ZOU	332.2–391.4	7	1.00	#	0.414	1.17−1	0.41	−7.13−2	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1886SCH	(4.46−1, 1.57, 3.90−1, 9)	1948TSC1	(3.80−2, 0.15, −3.80−2, −1)
1948TSC5	(5.25−2, 0.20, −5.25−2, −1)	1983GRO/FAR2	(4.78−2, 0.19, −4.78−2, −1)

Parameters of regression polynomial (14.29.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	56	44	0.425	5.71−2	0.20	−2.89−3	1

T/K	A_1	A_2	A_3	A_4	Uncert.
180.9–391.4	2.950 99+1	−1.105 57+1	4.611 93	−4.422 90−1	II

Parameters of quasipolynomial equation (14.29.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	56	41	0.471	6.67−2	0.23	1.02−3	2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
186.5–391.4	638.30	5.03662+2	5.09321+1	−2.98839+1	4.59697+2	1.38470+2	3.16000+2	II

Deviation plot for Propylbenzene (14-029) is given in Fig. 21.

6.2.4.10. Naphthalene (14-033)

Name:	Naphthalene
Formula:	$C_{10}H_8$
CAS-RN:	91-20-3
Group No:	14-033

Experimental heat capacities (14.33.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1890PIC		353.0–372.0	2		4.00	n/a	n/a	*p*	BDHO	1890PIC
1926AND/LYN	N	354.0–473.0	eqn		n/a	n/a	n/a	*p*	DSIO	1926AND/LYN
1931BLA/LEI		382.0–465.8	17		3.00	n/a	n/a	sat	BSIO	1931BLA/LEI
1932SPA/THO		363.1–463.1	11	S	1.00	n/a	n/a	*p*	BDHO	1931THO/PAR
1941SCH		353.0–473.0	eqn		n/a	n/a	n/a	*p*	n/a	n/a
1944EIB		353.0–473.0	eqn		n/a	n/a	n/a	*p*	n/a	n/a
1957MCC/FIN2		357.0–370.8	6		0.20	99.985	melpt	sat	BSAO	1947HUF
1964RAS/BAS		359.1	1		1.50	n/a	n/a	*p*	BSIO	1964RAS/BAS
1993CHI/KNI2		357.9–440.3	13		0.10	99.93	melpt	sat	BSAO	1988STE/ARC
1993CHI/KNI2		460.0–700.0	13		1.00	99.93	melpt	sat	BSAO	1988STE/ARC
1993DUR/AOU		373.0–473.0	102		n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1995DUR/AOU		373.0–473.0	eqn		2.00	99.	anal	*p*	BDCT	1986MER/BEN
2002CHI/KNI1		357.4–435.0	11		0.20	99.97	melpt	sat	BSAO	1988STE/ARC
2002VAN/VAN1		355.0–380.0	eqn		0.50	99.92	melpt	*p*	BSAO	2002VAN/VAN1

Reference	Notes
1926AND/LYN	calculated from temperature dependence of enthalpy by the compilers

6.2.4.11. Butylbenzene (14-036)

Name:	Butylbenzene
Formula:	$C_{10}H_{14}$
CAS-RN:	104-51-8
Group No:	14-036

Experimental heat capacities (14.36.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931HUF/PAR		191.9–298.2	8		1.00	n/a	n/a	*p*	BSIO	1925PAR
1948TSC1		293.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC5		295.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1965MES/TOD2		193.8–370.0	19		n/a	99.92	melpt	sat	BSAO	1947HUF
1983GRO/FAR3		298.1	1		0.30	99.	chrom	*p*	FSIT	1971PIC/LED
2002STE/CHI2		300.0–640.0	18	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2003PAR/ZOU		288.1–348.1	13		0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8		0.50	99.0	anal	sat	BDCT	1991BAN/GAR

Correlated heat capacities (14.36.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1965MES/TOD2	193.8–370.0	19	0.50	#	0.397	5.98−2	0.20	2.45−2	5
2002STE/CHI2	300.0–640.0	18	1.00		1.165	6.00−1	1.16	3.05−2	−2
2003PAR/ZOU	288.1–348.1	13	0.70	#	0.521	1.05−1	0.36	−7.64−2	−9
2006PAR/ZOU	332.2–401.3	8	0.70	#	0.405	9.24−2	0.28	−2.92−3	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1931HUF/PAR	(1.90−1, 0.67, −1.54−1, −7)	1948TSC1	(2.82−1, 0.99, −2.82−1, −1)
1948TSC5	(2.51−1, 0.87, −2.51−1, −1)	1983GRO/FAR3	(1.62−2, 0.06, 1.62−2, 1)

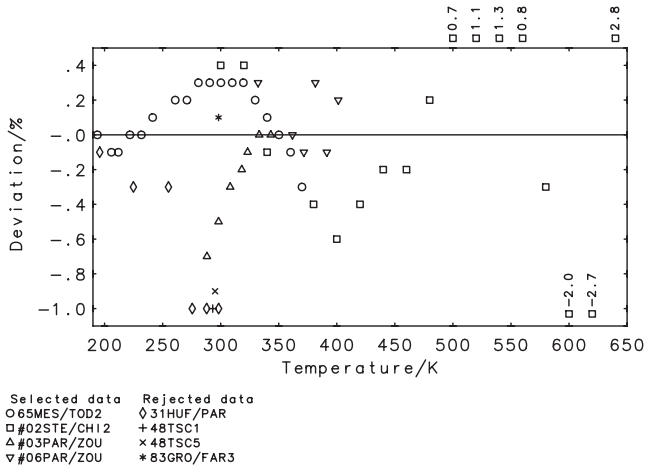

FIG. 22. Deviation plot for butylbenzene (14-036).

Parameters of cubic spline polynomials (14.36.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	69	58	0.780	3.57−1	0.72	−2.83−5	−8
sat	69	58	0.586	2.27−1	0.51	−4.61−3	−4

T/K	A_1	A_2	A_3	A_4	Uncert.
193.8–500.0	2.960 24+1	−8.148 34	3.560 54	−2.934 65−1	I
500.0–640.0	−4.607 51+2	2.860 64+2	−5.528 18+1	3.629 36	III
193.8–500.0	2.915 36+1	−7.707 96	3.424 76	−2.803 28−1	I
500.0–640.0	−2.653 81+2	1.690 13+2	−3.191 94+1	2.075 95	III

Parameters of quasipolynomial equation (14.36.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	69	58	1.402	4.01−1	1.03	1.42−2	−2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
193.8–640.0	660.50	−3.680 07	1.068 72−1	1.657 30+1	2.103 90+1	4.529 37	3.154 96−1	V

Deviation plot for Butylbenzene (14-036) is given in Fig. 22.

6.2.4.12. (1,1-Dimethylethyl)benzene (14-037)

Name:	(1,1-Dimethylethyl)benzene
Formula:	$C_{10}H_{14}$
CAS-RN:	98-06-6
Group No:	14-037

Experimental heat capacities (14.37.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930HUF/PAR1		220.4–294.3	8		1.00	n/a	n/a	p	BSIO	1925PAR
2002STE/CHI2		300.0–640.0	18	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2003PAR/ZOU		288.1–348.1	13		0.30	97.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8		1.00	97.0	anal	sat	BDCT	1991BAN/GAR

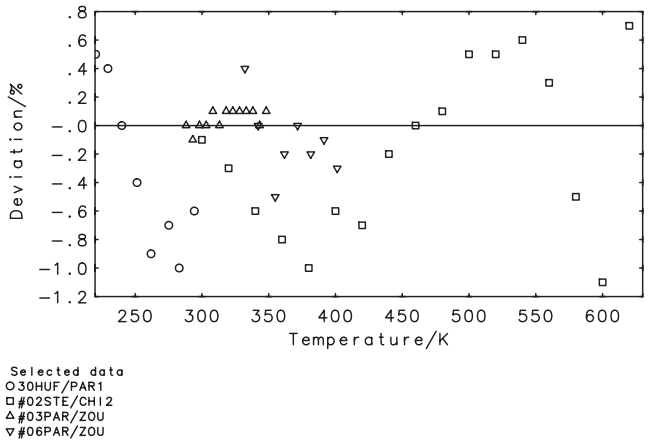

FIG. 23. Deviation plot for (1,1-dimethylethyl)benzene (14-037).

Correlated heat capacities (14.37.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1930HUF/PAR1	220.4–294.3	8	1.00	0.621	1.69−1	0.62	−9.37−2	−3
2002STE/CHI2	300.0–620.0	17	1.00	0.590	2.47−1	0.59	−5.81−2	−5
2003PAR/ZOU	288.1–348.1	13	0.30	0.221	2.03−2	0.07	1.46−2	10
2006PAR/ZOU	332.2–401.3	8	1.00	0.271	8.85−2	0.27	−3.71−2	−3

Parameters of cubic spline polynomials (14.37.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	47	46	0.499	1.81−1	0.48	−4.01−2	−1
sat	47	46	0.470	1.61−1	0.46	−3.90−2	4

T/K	A_1	A_2	A_3	A_4	Uncert.
220.4–520.0	1.997 30+1	−5.021 92−1	1.483 26	−9.949 57−2	II
520.0–620.0	−4.049 08+2	2.446 21+2	−4.565 59+1	2.922 24	IV
220.4–500.0	2.029 80+1	−8.641 92−1	1.614 31	−1.149 83−1	II
500.0–620.0	−2.933 64+1	2.891 65+1	−4.341 83	2.820 93−1	IV

Parameters of quasipolynomial equation (14.37.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	47	46	0.643	2.34−1	0.58	−5.96−3	10

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
220.4–620.0	647.30	−1.348 22	9.275 71−3	1.484 35+1	2.392 27+1	1.019 71+1	1.425 13	III

Deviation plot for (1,1–Dimethly)benzene (14-037) is given in Fig. 23.

6.2.4.13. (1-Methylpropyl)benzene (14-039)

Name:	(1-Methylpropyl)benzene
Formula:	$C_{10}H_{14}$
CAS-RN:	135-98-8
Group No:	14-039

Experimental heat capacities (14.39.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1979AND/GRI	N	293.7–429.6	9		0.80	n/a	n/a	sat	BSAO	1967RAS/GAN
2002STE/CHI2		300.0–640.0	18	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2003PAR/ZOU		288.1–348.1	13		0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8		0.50	99.0	anal	sat	BDCT	1991BAN/GAR

Reference	Notes
1979AND/GRI	error 0.5% below 373 K and 0.8% at 433 K

Correlated heat capacities (14.39.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1979AND/GRI	293.7–429.6	9	0.80	0.887	2.38−1	0.71	−1.89−1	−7
2002STE/CHI2	300.0–640.0	18	1.00	1.107	5.80−1	1.11	−3.20−2	−2
2003PAR/ZOU	288.1–348.1	13	0.30	0.755	7.16−2	0.23	2.57−2	−2
2006PAR/ZOU	332.2–401.3	8	0.50	0.422	6.89−2	0.21	−3.43−3	2

Parameters of cubic spline polynomials (14.39.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	48	48	0.940	3.94−1	0.80	−4.10−2	−9

T/K	A_1	A_2	A_3	A_4	Uncert.
288.1–565.0	1.455 30+1	4.912 28	−1.254 03−1	4.399 19−2	II
565.0–640.0	−6.089 12+3	3.245 80+3	−5.737 34+2	3.388 52+1	IV

Parameters of quasi-polynomial equation (14.39.4)

Type	nPts total	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	48	48	1.482	2.74−1	0.71	7.21−2	16

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
288.1–640.0	652.20	−4.063 56	2.300 64−1	1.032 60+1	3.958 16+1	−1.172 45+1	1.213 78	V

Deviation plot for (1–Methylpropyl)benzene (14-039) is given in Fig. 24.

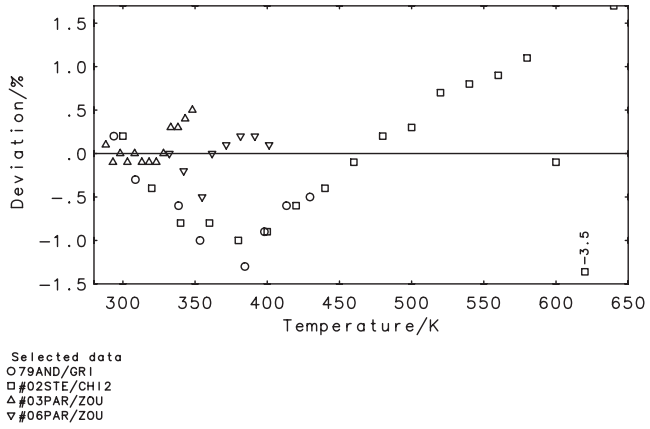

FIG. 24. Deviation plot for (1-methylpropyl)benzene (14-039).

6.2.4.14. 1,2,4,5-Tetramethylbenzene (14-042)

Name:	1,2,4,5-Tetramethylbenzene
Formula:	$C_{10}H_{14}$
CAS-RN:	95-93-2
Group No:	14-042

Experimental heat capacities (14.42.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1933FER/THO		363.1–393.1	4	S	n/a	n/a	n/a	p	BDHO	1931THO/PAR
1944EIB		352.0–473.0	eqn		n/a	n/a	n/a	p	n/a	n/a
1947KUR		382.8–413.8	3		n/a	n/a	n/a	avg	DSIO	1947KUR
2002VAN/VAN1		355.0–370.0	eqn		0.50	99.98	melpt	p	BSAO	2002VAN/VAN1

6.2.4.15. Hexylbenzene (14-060)

Name:	Hexylbenzene
Formula:	$C_{12}H_{18}$
CAS-RN:	1077-16-3
Group No:	14-060

Experimental heat capacities (14.60.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1948TSC1		293.1	1	n/a	n/a	n/a	p	BSIO	1948TSC1
1948TSC5		295.1	1	n/a	n/a	n/a	p	BSIO	1948TSC1
2003PAR/ZOU		288.1–323.1	8	0.30	97.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8	1.00	97.0	anal	sat	BDCT	1991BAN/GAR

Correlated heat capacities (14.60.2)

Reference	T/K	nPts	$\sigma_r C$/%	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2003PAR/ZOU	288.1–323.1	8	0.30			0.283	3.19−2	0.08	−5.20−3	0
2006PAR/ZOU	332.2–401.3	8	0.70		#	0.437	1.24−1	0.31	2.94−2	2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1948TSC1	(8.27−1, 2.34, −8.27−1, −1)	1948TSC5	(1.12, 3.18, −1.12, −1)	

Parameters of regression polynomial (14.60.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	18	16	0.408	1.01−1	0.25	1.21−2	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
288.1–401.3		2.634 52+1		3.664 53−1		1.010 54		II

Deviation plot for Hexylbenzene (14-060) is given in Fig. 25.

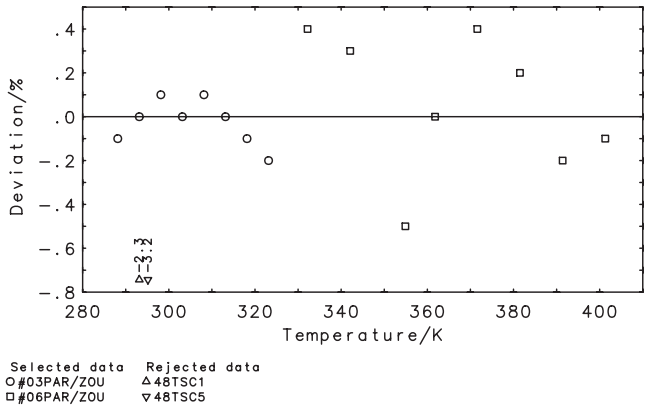

FIG. 25. Deviation plot for hexylbenzene (14-060).

6.2.4.16. 1,1′-Methylenebis(benzene) (14-062)

Name:	1,1′-Methylenebis(benzene)
Formula:	$C_{13}H_{12}$
CAS-RN:	101-81-5
Group No:	14-062

Experimental heat capacities (14.62.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1930HUF/PAR1		302.0–312.3	4		n/a	n/a	n/a	*p*	BSIO	1925PAR
1931BLA/LEI		308.1–368.1	13		n/a	n/a	n/a	*p*	BSIO	1931BLA/LEI
1931SMI/AND1		310.7–322.6	2		n/a	99.9	estim	*p*	DSIO	1926AND/LYN
1950KUR		313.8–414.4	8		n/a	n/a	n/a	avg	DSIO	1947KUR
1956DUF/EVE	N	303.1–353.1	6	S	n/a	n/a	n/a	*p*	n/a	n/a
2005CHI/STE2		303.4–438.4	12	S	0.20	99.98	melpt	sat	BSAO	1988STE/ARC
2005CHI/STE2		460.0–700.0	13	S	1.00	99.98	melpt	sat	BDHT	1989KNI/ARC

Reference	Notes
1956DUF/EVE	measured by a noncalorimetric method (piezothermometric)

Correlated heat capacities (14.62.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1930HUF/PAR1	302.0–312.3	4	1.00	#	0.928	3.01−1	0.93	−2.87−1	−4
2005CHI/STE2	303.4–438.4	12	0.70	#	0.355	8.65−2	0.25	6.41−2	7
2005CHI/STE2	460.0–700.0	13	1.00		0.447	2.36−1	0.45	−2.84−2	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1931BLA/LEI	(3.04, 7.94, 2.95, 13)	1931SMI/AND1	(3.04−1, 0.92, −9.79−2, 0)
1950KUR	(1.70, 4.50, 1.70, 8)	1956DUF/EVE	(7.74−1, 2.30, −7.37−1, −6)

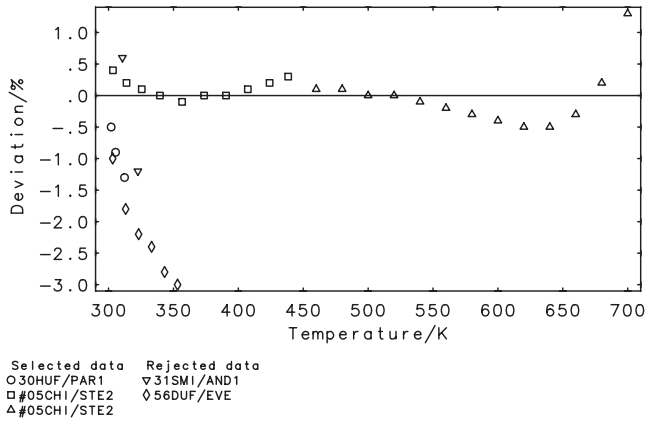

FIG. 26. Deviation plot for 1,1′-methylenebis(benzene) (14-062).

Parameters of regression polynomial (14.62.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	58	29	0.539	2.13−1	0.51	−2.57−2	0
sat	58	29	0.462	1.53−1	0.42	−2.00−2	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
302.0–700.0	9.683 45	8.335 47	−2.859 38−1		III
302.0–700.0	8.593 95	8.904 55	−3.574 68−1	III	

Parameters of quasipolynomial equation (14.62.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	58	29	0.500	1.42−1	0.41	6.87−3	1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
302.0–700.0	778.00	−2.122 96	8.005 44−2	5.164 62	8.317 27+1	−4.662 39+1	9.031 81	III

Deviation plot for 1,1′-Methylenebis(benzene) (14-062) is given in Fig. 26.

6.2.4.17. Heptylbenzene (14-065)

Name:	Heptylbenzene
Formula:	$C_{13}H_{20}$
CAS-RN:	1078-71-3
Group No:	14-065

Experimental heat capacities (14.65.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1948TSC1		294.1	1	n/a	n/a	n/a	p	BSIO	1948TSC1
1948TSC5		295.1	1	n/a	n/a	n/a	p	BSIO	1948TSC1
2003PAR/ZOU		288.1–348.1	13	0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8	0.50	99.0	anal	sat	BDCT	1991BAN/GAR

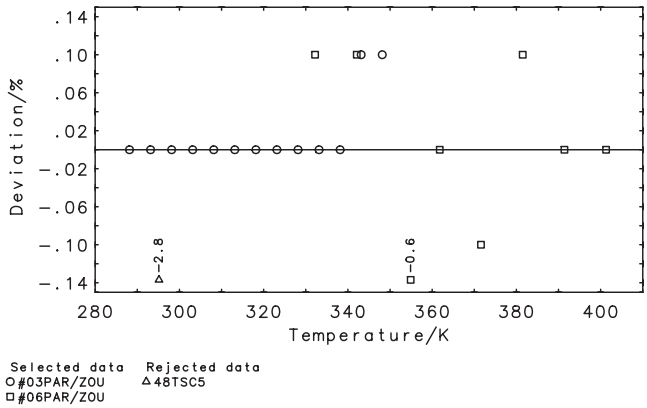

FIG. 27. Deviation plot for heptylbenzene (14-065).

Correlated heat capacities (14.65.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2003PAR/ZOU	288.1–348.1	13	0.30	0.131	1.69−2	0.04	5.72−3	2
2006PAR/ZOU	332.2–401.3	8	0.50	0.473	1.04−1	0.24	−2.53−2	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1948TSC1	(1.02, 2.62, −1.02, −1)	1948TSC5	(1.09, 2.80, −1.09, −1)

Parameters of regression polynomial (14.65.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	23	21	0.334	7.09−2	0.16	−6.08−3	3	
T/K		A_1		A_2		A_3	A_4	Uncert.
288.1–401.3		2.171 81+1		5.256 47		3.012 73−1		II

Deviation plot for Heptylbenzene (14-065) is given in Fig. 27.

6.2.4.18. Anthracene (14-066)

Name:	Anthracene
Formula:	$C_{14}H_{10}$
CAS-RN:	120-12-7
Group No:	14-066

Experimental heat capacities (14.66.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1917HIL/DUS	N	526.2–541.2	2	n/a	n/a	n/a	avg	DSIO	1911LEW/RAN
1970GOU/GIR	N	496.7–511.3	5	0.10	99.99	melpt	sat	BSAO	1953WES/HAT
1993DUR/AOU		492.0–592.0	51	n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1995DUR/AOU		492.0–592.0	eqn	2.00	99.9	anal	*p*	BDCT	1986MER/BEN
2003ROJ/ORO		495.0–503.0	10	n/a	99.95	melpt	*p*	BDHT	1995DIO/MAN

Reference	Notes
1917HIL/DUS	average values in the temperature ranges 489–563 and 489−593 K
1970GOU/GIR	smoothed value at 500 K in 1968GOU/GIR

6.2.4.19. 1,1′-(1,2-Ethynediyl)bis(benzene) (14-067)

Name:	1,1′-(1,2-Ethynediyl)bis(benzene)
Formula:	$C_{14}H_{10}$
CAS-RN:	501-65-5
Group No:	14-067

Experimental heat capacities (14.67.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1950KUR		364.5–552.5	10	n/a	n/a	n/a	avg	DSIO	1947KUR
2002STE/CHI3		335.0–500.0	eqn	1.00	99.8	chrom	sat	BDHT	1989KNI/ARC

6.2.4.20. Phenanthrene (14-068)

Name:	Phenanthrene
Formula:	$C_{14}H_{10}$
CAS-RN:	85-01-8
Group No:	14-068

Experimental heat capacities (14.68.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1941SCH		371.0–473.0	eqn	n/a	n/a	n/a	*p*	n/a	n/a
1944EIB		371.0–473.0	eqn	n/a	n/a	n/a	*p*	n/a	n/a
1964RAS/BAS		379.1	1	1.50	n/a	n/a	*p*	BSIO	1964RAS/BAS
1977FIN/MES		383.3–408.6	4	0.20	99.987	melpt	sat	BSAO	1947HUF
1993DUR/AOU		392.0–492.0	51	n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1995DUR/AOU		392.0–492.0	eqn	2.00	98.0	anal	*p*	BDCT	1986MER/BEN
2003ROJ/ORO		382.0–393.0	12	n/a	99.97	melpt	*p*	BDHT	1995DIO/MAN

6.2.4.21. Pyrene (14-079)

Name:	Pyrene
Formula:	$C_{16}H_{10}$
CAS-RN:	129-00-0
Group No:	14-079

Experimental heat capacities (14.79.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1971WON/WES		430.6–478.8	7	0.10	99.97	melpt	sat	BSAO	1968WES/WES
1993DUR/AOU		492.0–592.0	51	n/a	n/a	n/a	*p*	BDCT	1986MER/BEN
1995DUR/AOU		492.0–592.0	eqn	2.00	99.0	anal	*p*	BDCT	1986MER/BEN
2003ROJ/ORO		427.0–443.1	18	n/a	99.96	melpt	*p*	BDHT	1995DIO/MAN

6.2.4.22. (4*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene (14-105)

Name:	(4*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene
Formula:	$C_{10}H_{16}$
CAS-RN:	5989-27-5
Group No:	14-105

Experimental heat capacities (14.105.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996GAL/VAN1		202.0–250.1	24		0.20	99.31	melpt	p	BSAO	1987VAN/VAN
2002STE/CHI1		300.0–620.0	17	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (14.105.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1996GAL/VAN1	202.0–250.1	24	0.20	0.854	4.41−2	0.17	−4.67−4	−4
2002STE/CHI1	300.0–620.0	17	1.00	0.494	2.16−1	0.49	2.41−2	2

Parameters of cubic spline polynomials (14.105.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	41	41	0.776	1.53−1	0.37	9.73−3	−2
sat	41	41	0.759	1.23−1	0.34	1.03−2	−4

T/K	A_1	A_2	A_3	A_4	Uncert.
202.0–450.0	4.316 32+1	−2.168 59+1	7.924 80	−7.150 16−1	II
450.0–620.0	−2.524 98+2	1.754 21+2	−3.587 68+1	2.529 55	IV
202.0–450.0	4.281 15+1	−2.130 18+1	7.791 43	−7.006 50−1	II
450.0–620.0	−2.076 23+2	1.456 55+2	−2.931 00+1	2.047 60	IV

Parameters of quasi-polynomial equation (14.105.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	41	17	0.199	9.20−2	0.20	1.43−4	1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
300.0–620.0	655.00	−3.373 06	4.555 12−1	−1.288 74	8.450 40+1	−5.430 23+1	1.291 58+1	III

Deviation plot for (4*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene (14-105) is given in Fig. 28.

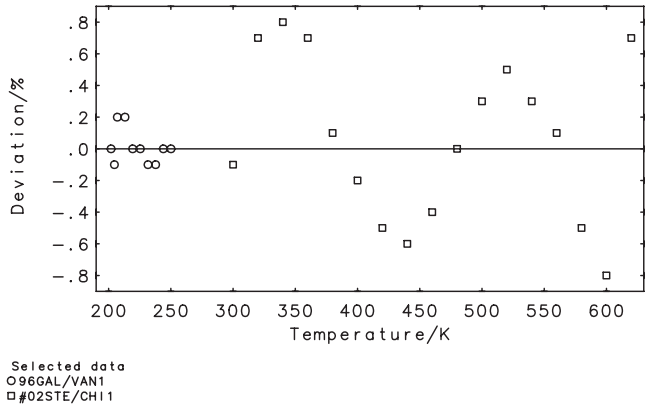

FIG. 28. Deviation plot for (4*R*)-1-methyl-4-(1-methylethenyl)cyclohexene (14-105).

6.2.4.23. 1,4-Bis(1-methylethyl)benzene (14-110)

Name:	1,4-Bis(1-methylethyl)benzene
Formula:	$C_{12}H_{18}$
CAS-RN:	100-18-5
Group No:	14-110

Experimental heat capacities (14.110.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1998VER2		298.1	1		n/a	99.92	chrom	p	BDHT	1969PER/COM
2002STE/CHI5		300.0–640.0	17	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (14.110.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002STE/CHI5	300.0–640.0	17	1.00	0.283	1.64−1	0.28	1.06-3	1

Parameters of cubic spline polynomials (14.110.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	18	17	0.337	1.96−1	0.34	1.06−3	1
sat	18	17	0.223	1.26−1	0.22	4.42−4	1

T/K	A_1	A_2	A_3	A_4	Uncert.
300.0–510.0	2.037 80+1	1.645 23	1.56001	−1.412 12−1	II
510.0–640.0	−3.587 32+2	2.246 51+2	−4.216 66+1	2.716 74	III
300.0–510.0	1.761 84+1	3.687 00	1.07229	−1.038 14−1	I
510.0–640.0	−2.156 32+2	1.408 93+2	−2.583 08+1	1.654 56	III

Parameters of quasipolynomial equation (14.110.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	18	17	0.195	1.02−1	0.19	3.95−4	−2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
300.0–640.0	675.00	−3.545 76	2.267 62−1	4.984 63	8.051 28+1	−4.336 14+1	8.271 75	I

Deviation plot for 1,4–Bis(methylethyl)benzene (14-110) is given in Fig. 29.

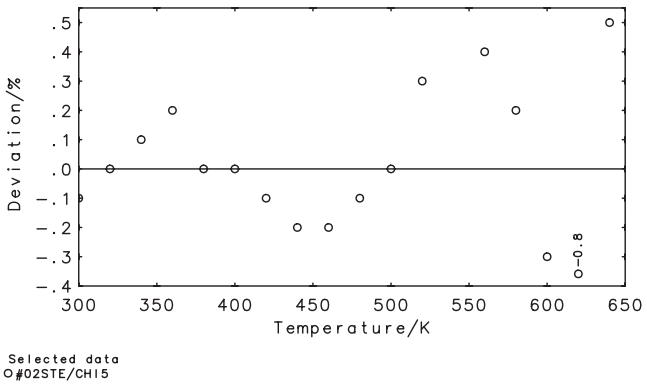

FIG. 29. Deviation plot for 1,4-bis(1-methylethyl)benzene (14-110).

6.2.4.24. 5-Ethylidenebicyclo[2.2.1]hept-2-ene (14-126)

Name:	5-Ethylidenebicyclo[2.2.1]hept-2-ene
Formula:	C_9H_{12}
CAS-RN:	16219-75-3
Group No:	14-126

Experimental heat capacities (14.126.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005BYK/NIK		134.3–348.1	130	0.20	99.5	anal	p	BSAO	1997VAR/DRU1

Correlated heat capacities (14.126.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2005BYK/NIK	134.3–348.1	130	1.00	0.205	4.65−2	0.21	1.18−3	−3

Parameters of regression polynomial (14.126.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	130	130	0.204	4.60−2	0.20	1.71−4	−8

T/K	A_1	A_2	A_3	A_4	Uncert.
134.3–348.1	2.774 28+1	−1.329 36+1	5.970 59	−6.443 03−1	III

Deviation plot for 5–Ethylidenebicyclo[2.2.1]hept–2–ene (14-126) is given in Fig. 30.

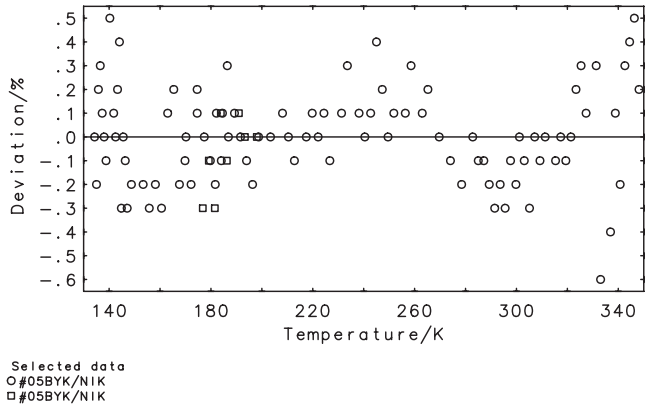

FIG. 30. Deviation plot for 5-ethylidenebicyclo[2.2.1]hept-2-ene (14-126).

6.2.4.25. (2-Methylpropyl)benzene (14-127)

Name:	(2-Methylpropyl)benzene
Formula:	$C_{10}H_{14}$
CAS-RN:	538-93-2
Group No:	14-127

Experimental heat capacities (14.127.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003PAR/ZOU		288.1–348.1	13	0.30	99.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8	0.50	99.0	anal	sat	BDCT	1991BAN/GAR

Correlated heat capacities (14.127.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2003PAR/ZOU	288.1–348.1	13	0.30	0.142	1.32−2	0.04	6.73−3	5
2006PAR/ZOU	332.2–401.3	8	0.50	0.486	7.93−2	0.24	−2.99−2	−2

Parameters of regression polynomial (14.127.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
sat	21	21	0.345	5.40−2	0.17	−7.23−3	3	
T/K		A_1		A_2		A_3	A_4	Uncert.
288.1–401.3		1.369 11+1		4.675 41		1.772 55−1		II

Deviation plot for (2–Methylpropyl)benzene (14-127) is given in Fig. 31.

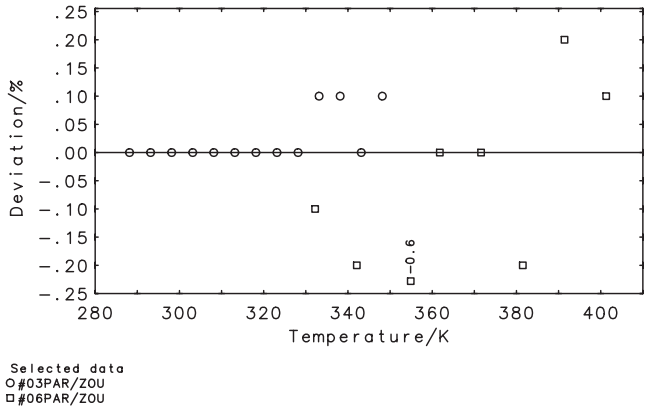

FIG. 31. Deviation plot for (2-methylpropyl)benzene (14-127).

6.2.4.26. (1*R*,5*R*)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (14-128)

Name: (1*R*,5*R*)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene

Formula: $C_{10}H_{16}$
CAS-RN: 7785-70-8
Group No: 14-128

Experimental heat capacities (14.128.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005FUJ/MAT		293.1–308.1	4	n/a	99.99	chrom	*p*	BDHT	2005FUJ/MAT

Parameters of regression polynomial (14.128.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.012	3.49−3	0.01	4.77−7	1
T/K		A_1		A_2	A_3	A_4	Uncert.
293.1–308.1		1.471 91+1		5.104 66			III

6.2.4.27. (1*S*,5*S*)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (14-129)

Name: (1*S*,5*S*)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene

Formula: $C_{10}H_{16}$
CAS-RN: 7785-26-4
Group No: 14-129

Experimental heat capacities (14.129.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005FUJ/MAT		293.1–308.1	4	n/a	99.99	chrom	*p*	BDHT	2005FUJ/MAT

Parameters of regression polynomial (14.129.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.018	5.53−3	0.02	9.54−7	0
T/K		A_1		A_2	A_3	A_4	Uncert.
293.1–308.1		1.489 54+1		5.044 92			III

6.2.4.28. 1,4-Bis(1,1-dimethylethyl)benzene (14-130)

Name: 1,4-Bis(1,1-dimethylethyl)benzene

Formula: $C_{14}H_{22}$
CAS-RN: 1012-72-2
Group No: 14-130

Experimental heat capacities (14.130.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997STE/CHI3		360.0–680.0	17	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of cubic spline polynomials (14.130.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	17	17	0.350	2.56−1	0.35	1.48−3	1

T/K	A_1	A_2	A_3	A_4	Uncert.
360.0–550.0	−8.536 03	2.172 59+1	−1.990 59	7.659 24−2	II
550.0–680.0	−7.206 08+2	4.101 29+2	−7.260 93+1	4.356 51	III

6.2.4.29. 1,2,4,5-Tetrakis(1-methylethyl)benzene (14-131)

Name:	1,2,4,5-Tetrakis(1-methylethyl)benzene

Formula:	$C_{18}H_{30}$
CAS-RN:	635-11-0
Group No:	14-131

Experimental heat capacities (14.131.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI5		410.0–690.0	15	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of cubic spline polynomials (14.131.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	15	15	0.720	6.85−1	0.72	7.28−3	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
410.0–580.0	2.172 77+2	−1.079 33+2	2.438 37+1	−1.665 39	II
580.0–690.0	−2.471 00+3	1.282 56+3	−2.153 56+2	1.211 27+1	III

6.2.4.30. 1,1′,1″-(1-Ethenyl-2-ylidine)tris(benzene) (14-132)

Name:	1,1′,1″-(1-Ethenyl-2-ylidine)tris(benzene)

Formula:	$C_{20}H_{16}$
CAS-RN:	58-72-0
Group No:	14-132

Experimental heat capacities (14.132.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1998HIK/OKA		340.4–354.2	7	0.30	99.995	melpt	p	BSAO	1993FUJ/OGU1

Parameters of regression polynomial (14.132.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.077	1.24−2	0.02	2.73−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
340.4–354.2	2.365 63+1	8.753 73			II

6.2.4.31. Hexadecylbenzene (14-133)

Name:	Hexadecylbenzene
Formula:	$C_{22}H_{38}$
CAS-RN:	1459-09-2
Group No:	14-133

Experimental heat capacities (14.133.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003PAR/ZOU		303.1–348.1	10	0.30	97.0	anal	sat	BDCT	1983ROU/ROU
2006PAR/ZOU		332.2–401.3	8	1.00	97.0	anal	sat	BDCT	1991BAN/GAR

Correlated heat capacities (14.133.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2003PAR/ZOU	303.1–348.1	10	0.30	0.069	1.60−2	0.02	−2.84−3	−2
2006PAR/ZOU	332.2–401.3	8	1.00	0.162	1.31−1	0.16	4.00−2	2

Parameters of regression polynomial (14.133.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
sat	18	18	0.131	9.66−2	0.12	1.62−2	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
303.1–401.3		7.715 88+1		−1.204 50+1		3.602 38		II

6.3. Main group 2: compounds of carbon, hydrogen, and halogens

6.3.1. Subgroup 21: fluorinated hydrocarbons

6.3.1.1. Trifluoromethane (21-002)

Name:	Trifluoromethane
Formula:	CHF_3
CAS-RN:	75-46-7
Group No:	21-002

Experimental heat capacities (21.2.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1962VAL/BRO		122.7–189.3	8	n/a	99.999	melpt	sat	BSIO	1937GIA/EGA
1972COP/REA		127.6–142.9	4	n/a	99.8	chrom	*p*	BSAO	1968WES/FUR
1978SOL/SUK		123.0–153.0	eqn	n/a	n/a	n/a	sat	BSAO	1978SOL/SUK
1978SOL/SUK		153.0–288.0	eqn	n/a	n/a	n/a	sat	BSAO	1978SOL/SUK
1984STO/CHA		173.0–191.0	eqn	0.30	99.98	anal	*p*	BSAO	1978SOL/SUK
2000MAG/DUA		120.6–295.1	94	0.70	99.9999	anal	sat	BSAO	1961GOO

Correlated heat capacities (21.2.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1962VAL/BRO	122.7–189.3	8	0.50	#	0.297	1.53−2	0.15	−3.68−3	1
1972COP/REA	127.6–142.9	4	0.50	#	0.337	1.70−2	0.17	−1.11−2	−2
1978SOL/SUK	123.0–153.0	6	0.50	#	0.159	8.04−3	0.08	−5.37−3	−4

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1978SOL/SUK	153.0–287.4	15	1.00	#	0.634	1.09−1	0.63	−1.64−2	−7
1984STO/CHA	173.0–191.0	5	0.50	#	0.086	4.41−3	0.04	2.84−3	2
2000MAG/DUA	120.6–293.2	93	1.00	#	0.600	1.22−1	0.60	8.91−3	25

Parameters of cubic spline polynomials (21.2.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	132	131	0.572	1.12−1	0.56	3.74−3	15
sat	131	130	0.451	7.77−2	0.44	2.94−3	10

T/K	A_1	A_2	A_3	A_4	Uncert.
120.6–220.0	1.427 43+1	−5.876 12	2.129 35	−5.571 50−2	III
220.0–275.0	−1.556 31+2	2.258 13+2	−1.031 84+2	1.590 08+1	III
275.0–293.2	−3.333 69+4	3.642 36+4	−1.326 60+4	1.611 39+3	IV
120.6–220.0	1.421 74+1	−5.936 62	2.292 76	−1.199 77−1	III
220.0–275.0	−9.598 37+1	1.443 38+2	−6.601 37+1	1.022 95+1	III
275.0–293.2	−2.188 09+4	2.390 97+4	−8.707 98+3	1.057 74+3	IV

Parameters of quasipolynomial equation (21.2.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	131	130	0.528	5.22−2	0.40	−3.97−3	−11

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
120.6–293.2	299.30	−2.345 26	3.095 79−1	9.322 30	1.109 79	−1.149 51+1	7.066 22	III

Deviation plot for Trifluoromethane (21–002) is given in Fig. 32.

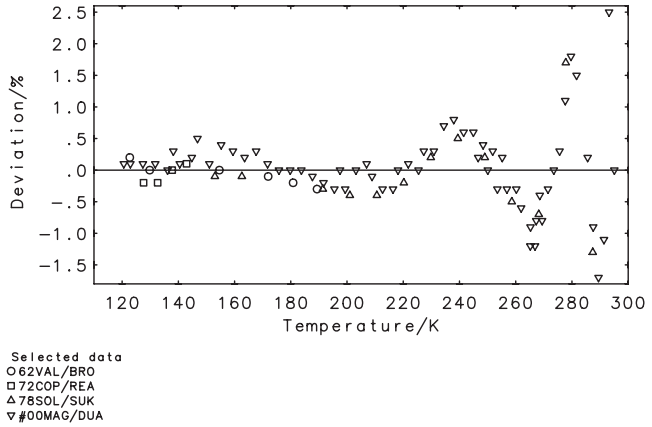

FIG. 32. Deviation plot for trifluoromethane (21-002).

6.3.1.2. Hexafluorobenzene (21-010)

Name:	Hexafluorobenzene
Formula:	C_6F_6
CAS-RN:	392-56-3
Group No:	21-010

Experimental heat capacities (21.10.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1965COU/GRE		281.9–305.9	8	0.20	99.97	melpt	*p*	BSAO	1963AND/COU1
1970MES/FIN		284.8–342.7	8	0.20	99.93	melpt	sat	BSAO	1947HUF
1982GOR/SIM1	N	284.0–349.7	18	0.50	99.74	melpt	*p*	FSIO	1983GOR/SIM
1982GOR/SIM2		279.0–353.0	eqn	n/a	99.9	anal	*p*	FSIO	1983GOR/SIM
1987WIL/LAI		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1995WIL/ING		298.1	1	n/a	99.0	chrom	*p*	FSIT	1971PIC/LED

Reference	Notes
1982GOR/SIM1	same data in 1982GOR/GRI

6.3.1.3. 3,5-Difluoro-4′-propyl-1,1′-biphenyl (21-057)

Name:	3,5-Difluoro-4′-propyl-1,1′-biphenyl
Formula:	$C_{15}H_{14}F_2$
CAS-RN:	137528-87-1
Group No:	21-057

Experimental heat capacities (21.57.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004ZOU/TAN		300.5–329.7	15	0.40	99.7	melpt	*p*	BSAO	1995TAN/SUN

Parameters of regression polynomial (21.57.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	15	15	0.197	3.40−2	0.08	4.09−5	−5		
T/K		A_1		A_2		A_3		A_4	Uncert.
300.5–329.7		−1.399 04+2		1.019 89+2		−1.387 00+1			II

6.3.2. Subgroup 22: chlorinated hydrocarbons

6.3.2.1. Tetrachloroethene (22-005)

Name:	Tetrachloroethene
Formula:	C_2Cl_4
CAS-RN:	127-18-4
Group No:	22-005

Experimental heat capacities (22.5.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		317.7–346.1	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1913HER/RAT		293.1	1		n/a	n/a	n/a	*p*	DSIO	1922HER/SCH
1948KUR		319.3–340.9	2		n/a	n/a	n/a	avg	DSIO	1947KUR
1966SAV		293.0–333.0	eqn		1.20	n/a	n/a	*p*	BSIO	1966SAV
1982GRO/ING		298.1	1		0.30	99.	estim	*p*	FSIT	1971PIC/LED
1986NOV/RAB		253.1–300.0	14		0.30	99.77	melpt	*p*	BSAO	1976LEB/LIT
1989WIL/LAI		298.1	1		n/a	99.7	anal	*p*	FSIT	1971PIC/LED
2000TAK/TAM		298.1	1		n/a	99.99	chrom	*p*	FSIO	1985OGA

6.3.2.2. 1,2-Dichloroethane (22-018)

Name:	1,2-Dichloroethane
Formula:	$C_2H_4Cl_2$
CAS-RN:	107-06-2
Group No:	22-018

Experimental heat capacities (22.18.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1912SCH1		293.1–323.1	3		n/a	n/a	n/a	*p*	BSIO	1912SCH1
1939RAI	N	240.0–322.0	15		2.00	99.96	melpt	*p*	BDHO	1937STU
1940PIT1		238.7–307.5	6		0.20	99.942	melpt	*p*	BSIO	1928LAT/GRE
1948KUR		270.5–322.1	4		n/a	n/a	n/a	avg	DSIO	1947KUR
1948TSC5		294.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1948TSC6		294.1	1		n/a	n/a	n/a	*p*	BSIO	1948TSC1
1949TSC/RIC3		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1951SIE/CRU	N	293.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1955RUI2		280.8–323.7	4		n/a	n/a	n/a	*p*	BSIO	1955RUI1
1955STA/TUP		284.1–348.0	14		1.00	n/a	n/a	*p*	BSAO	1955STA/TUP
1967RAS/GAN		293.1–353.1	4	S	0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1969WIL/SCH		293.1–313.1	3		0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1977WIL/GRO		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1979WIL/FAR		298.1	1		0.30	99.5	melpt	*p*	FSIT	1971PIC/LED
1979WIL/GRO		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1985LAI/ROU		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1989PRA/RAJ		318.1–333.1	4		3.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1993HAL		298.1	1		0.15	99.9	chrom	*p*	DDCT	1974SUU/WAD
1993SHE		308.1	1		n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
2003GOR/TKA		284.2–353.1	30		0.15	99.5	chrom	*p*	BDCT	2000ERN/CHO

Reference	Note
1939RAI	data from a graph only
1951SIE/CRU	heat of mixing calorimeter used

Correlated heat capacities (22.18.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1940PIT1	238.7–307.5	5	0.20		0.791	2.42−2	0.16	−3.67−3	−1
1955RUI2	280.8–323.7	4	1.00	#	0.578	9.14−2	0.58	6.69−2	3
1955STA/TUP	284.1–343.2	13	1.00		1.141	1.84−1	1.14	1.35−1	9
1967RAS/GAN	293.1–353.1	4	1.00	#	0.679	1.08−1	0.68	1.05−1	4

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1969WIL/SCH	293.1–313.1	3	1.00	#	0.491	7.63−2	0.49	−7.17−2	−3
1977WIL/GRO	298.1	1	0.30		0.136	6.32−3	0.04	−6.32−3	−1
1979WIL/FAR	298.1	1	0.30		0.136	6.32−3	0.04	−6.32−3	−1
1979WIL/GRO	298.1	1	0.30		0.239	1.11−2	0.07	−1.11−2	−1
1985LAI/ROU	298.1	1	0.30	#	0.602	2.80−2	0.18	−2.80−2	−1
1993SHE	308.1	1	0.50	#	0.379	2.96−2	0.19	2.96−2	1
2003GOR/TKA	284.2–353.1	30	0.15		0.264	6.30−3	0.04	−9.24−4	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1912SCH1	(3.44−1, 2.28, −3.06−1, −3)	1939RAI	(3.08−1, 2.05, 2.32−2, 3)
1948KUR	(7.63−1, 5.39, −6.23−1, −4)	1948TSC5	(1.96−1, 1.28, −1.96−1, −1)
1948TSC6	(1.71−1, 1.12, −1.71−1, −1)	1949TSC/RIC3	(5.15−1, 3.21, 5.15−1, 1)
1951SIE/CRU	(5.39−1, 3.61, −5.39−1, −1)	1989PRA/RAJ	(7.97−1, 5.30, −7.96−1, −4)
1993HAL	(4.30−2, 0.28, 4.30−2, 1)		

Parameters of regression polynomial (22.18.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	97	64	0.661	9.44−2	0.59	3.38−2	12	
T/K		A_1		A_2		A_3	A_4	Uncert.
238.7–353.1		1.657 41+1		−1.639 20		4.312 38−1		III

Parameters of quasipolynomial equation (22.18.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−				
p	97	66	2.027	1.10−1	0.70	1.76−2	−6				
T/K		T_c/K	A_1		A_2		A_3	A_4	A_5	A_6	Uncert.
238.7–353.1		561.60	−2.282 63−1		1.868 75−3		1.164 03+1	6.970 47			IV

Deviation plot for 1,2–Dichloroethane (22–018) is given in Fig. 33.

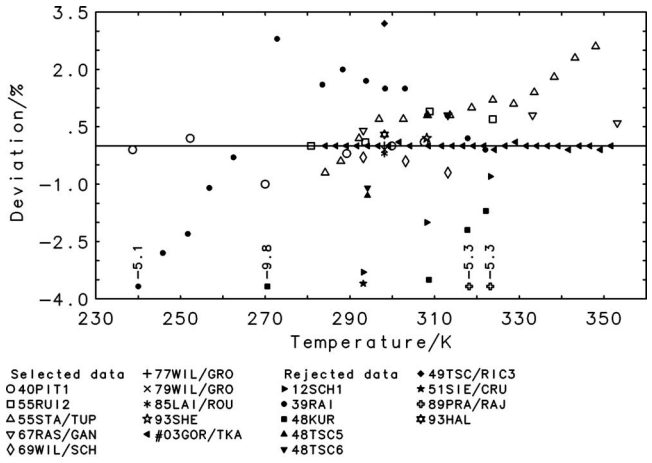

FIG. 33. Deviation plot for 1,2-dichloroethane (22-018).

6.3.2.3. 1,3-Dichloropropane (22-024)

Name:	1,3-Dichloropropane
Formula:	$C_3H_6Cl_2$
CAS-RN:	142-28-9
Group No:	22-024

Experimental heat capacities (22.24.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993HAL		298.1	1	0.15	99.9	chrom	p	DDCT	1974SUU/WAD
1993SHE		308.1	1	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2002GON/TOV		283.1–323.1	6	n/a	99.8	chrom	p	BDCT	1970PAZ/PAZ
2003GOR/TKA		284.2–353.1	30	0.15	99.5	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.24.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993HAL	298.1	1	0.15		0.221	6.26−3	0.03	−6.26−3	−1
1993SHE	308.1	1	0.50	#	0.249	2.37−2	0.12	2.37−2	1
2002GON/TOV	283.1–323.1	6	0.50	#	0.331	3.16−2	0.17	−1.24−2	−2
2003GOR/TKA	284.2–353.1	30	0.15		0.335	9.76−3	0.05	3.72−4	1

Parameters of regression polynomial (22.24.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	38	38	0.344	1.64−2	0.09	−1.20−3	−1	
T/K		A_1		A_2		A_3	A_4	Uncert.
283.1–353.1		1.595 55+1		1.313 45−1		2.859 48−1		II

Deviation plot for 1,3–Dichloropropane (22–024) is given in Fig. 34.

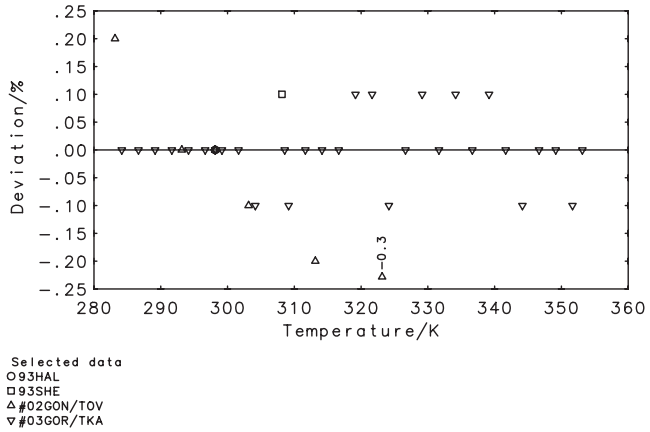

FIG. 34. Deviation plot for 1,3-dichloropropane (22-024).

6.3.2.4. 1-Chloropropane (22-026)

Name:	1-Chloropropane
Formula:	C_3H_7Cl
CAS-RN:	540-54-5
Group No:	22-026

Experimental heat capacities (22.26.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		299.1–311.6	4	S	n/a	n/a	n/a	avg	DSIO	1881VON
1948EUC	N	200.0–293.0	4	S	n/a	n/a	n/a	*p*	n/a	n/a
1948KUR		261.9–300.8	2		n/a	n/a	n/a	avg	DSIO	1947KUR
2005CHO/GOR		284.1–314.1	13		0.15	99.0	chrom	*p*	BDCT	2000ERN/CHO

Reference	Notes
1948EUC	unpublished data measured by A. Landsberg

Correlated heat capacities (22.26.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1881VON	299.1–311.6	4	1.00	#	0.423	6.74−2	0.42	4.40−2	2
1948EUC	200.0–293.0	3	2.00	#	0.640	1.90−1	1.28	−9.49−2	1
2005CHO/GOR	284.1–314.1	13	0.50	#	0.143	1.13−2	0.07	−1.88−3	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

Reference	
1948KUR	(7.86−2, 0.49, 5.37−2, 0)

Parameters of regression polynomial (22.26.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	23	20	0.361	8.69−2	0.58	−6.66−3	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
200.0–314.1	5.025 40	4.858 63	−4.181 94−1		III

Parameters of quasipolynomial equation (22.26.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	23	20	0.438	8.23−2	0.55	−6.18−3	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
200.0–314.1	503.00	4.475 68	2.267 20−1	6.164 28	2.208 86+1			IV

Deviation plot for 1–Chloropropane (22–026) is given in Fig. 35.

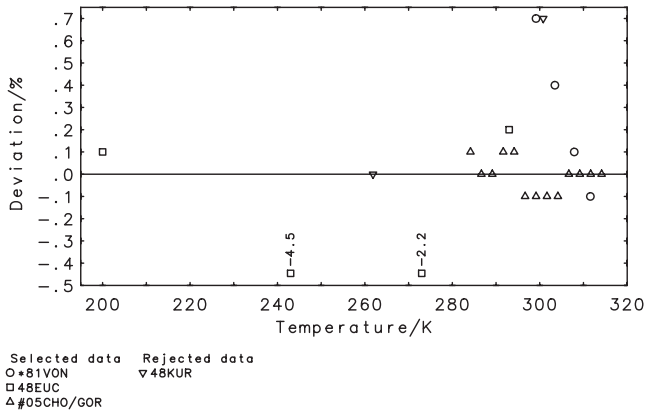

FIG. 35. Deviation plot for 1-chloropropane (22-026).

6.3.2.5. 1,4-Dichlorobutane (22-028)

Name:	1,4-Dichlorobutane
Formula:	$C_4H_8Cl_2$
CAS-RN:	110-56-5
Group No:	22-028

Experimental heat capacities (22.28.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1985LAI/WIL		298.1	1	0.30	99.5	estim	p	FSIT	1971PIC/LED
1993HAL		298.1	1	0.15	99.9	chrom	p	DDCT	1974SUU/WAD
1993SHE		308.1	1	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2003GOR/TKA		284.2–353.1	30	0.15	99.5	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.28.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1985LAI/WIL	298.1	1	0.30		0.355	2.35−2	0.11	−2.35−2	−1
1993HAL	298.1	1	1.00	#	0.117	2.58−2	0.12	2.58−2	1
1993SHE	308.1	1	2.00	#	0.480	2.16−1	0.96	2.16−1	1
2003GOR/TKA	284.2–353.1	30	0.15		0.259	8.86−3	0.04	1.44−4	3

Parameters of regression polynomial (22.28.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	33	33	0.282	4.10−2	0.18	6.75−3	4

T/K	A_1	A_2	A_3	A_4	Uncert.
284.2–353.1	1.836 95+1	2.350 05−1	3.413 25−1		III

Deviation plot for 1,4–Dichlorobutane (22–028) is given in Fig. 36.

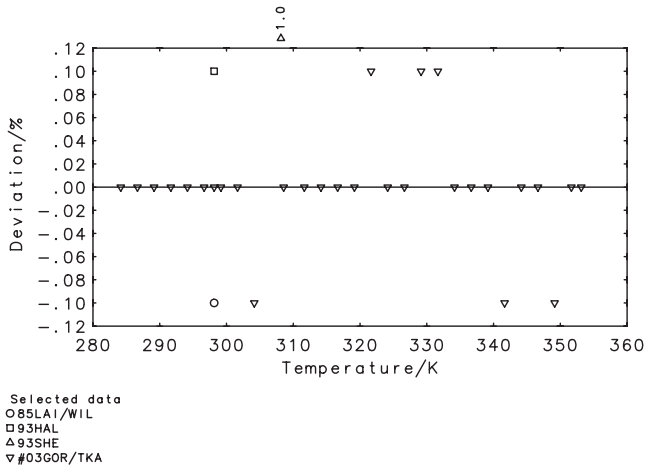

FIG. 36. Deviation plot for 1,4-dichlorobutane (22-028).

6.3.2.6. 1-Chlorobutane (22-029)

Name:	1-Chlorobutane
Formula:	C_4H_9Cl
CAS-RN:	109-69-3
Group No:	22-029

Experimental heat capacities (22.29.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1961ROU		300.9–309.0	12	n/a	n/a	n/a	p	BSAO	1961ROU
1985LAI/WIL		298.1	1	0.30	99.5	estim	p	FSIT	1971PIC/LED
1993GRO/ROU		298.1	1	n/a	99.5	anal	p	FSIT	1971PIC/LED
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.29.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1985LAI/WIL	298.1	1	1.00	#	0.274	5.26−2	0.27	5.26−2	1
1993GRO/ROU	298.1	1	0.50	#	0.410	3.94−2	0.21	3.94−2	1
1993SHE	298.1–308.1	2	0.50	#	0.272	2.60−2	0.14	−1.57−2	0
2005CHO/GOR	284.1–353.1	29	0.50	#	0.225	2.30−2	0.11	−6.62−4	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1961ROU	(3.46−1, 1.76, 3.38−1, 12)

Parameters of regression polynomial (22.29.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	45	33	0.249	2.64−2	0.13	1.25−3	3

T/K	A_1	A_2	A_3	A_4	Uncert.
284.1–353.1	1.695 74+1	−1.180 65	6.423 85−1		II

Deviation plot for 1–Chlorobutane (22–029) is given in Fig. 37.

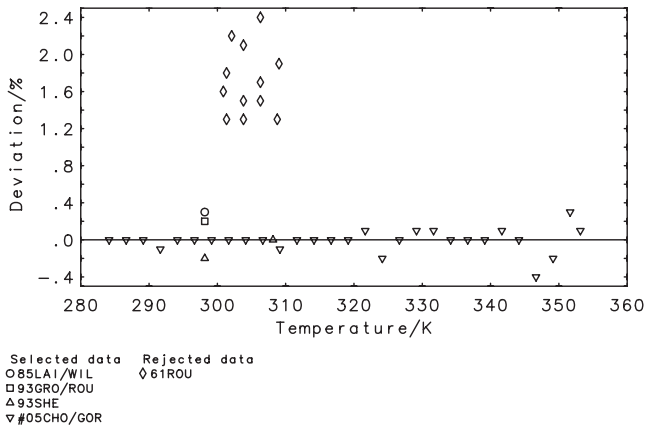

FIG. 37. Deviation plot for 1-chlorobutane (22-029).

6.3.2.7. 1,5-Dichloropentane (22-033)

Name:	1,5-Dichloropentane
Formula:	$C_5H_{10}Cl_2$
CAS-RN:	628-76-2
Group No:	22-033

Experimental heat capacities (22.33.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993HAL		298.1	1	0.15	99.9	chrom	p	DDCT	1974SUU/WAD
1993SHE		308.1	1	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2003GOR/TKA		284.2–353.1	30	0.15	99.5	chrom	p	BDCT	2000ERN/CHO
2004GON/PEL		283.1–323.1	9	n/a	99.1	chrom	p	BDCT	1970PAZ/PAZ

Correlated heat capacities (22.33.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993HAL	298.1	1	2.00	#	0.161	8.29−2	0.32	8.29−2	1
1993SHE	308.1	1	1.00	#	0.499	1.30−1	0.50	1.30−1	1
2003GOR/TKA	284.2–353.1	30	0.15		0.312	1.24−2	0.05	−6.13−4	−2
2004GON/PEL	283.1–323.1	9	0.50	#	0.227	2.88−2	0.11	1.90−2	5

Parameters of regression polynomial (22.33.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	41	41	0.310	3.07−2	0.12	8.91−3	5	
T/K		A_1		A_2		A_3	A_4	Uncert.
283.1–353.1		2.134 06+1		−5.504 10−3		4.791 18−1		III

Deviation plot for 1,5–Dichloropentane (22–033) is given in Fig. 38.

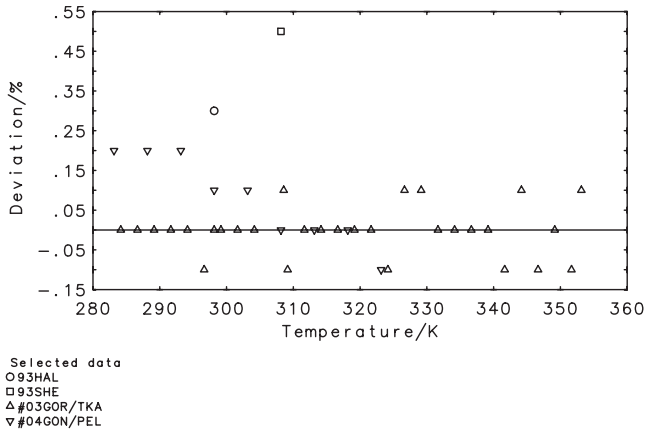

FIG. 38. Deviation plot for 1,5-dichloropentane (22-033).

6.3.2.8. 1,2,4-Trichlorobenzene (22-035)

Name:	1,2,4-Trichlorobenzene
Formula:	$C_6H_3Cl_3$
CAS-RN:	120-82-1
Group No:	22-035

Experimental heat capacities (22.35.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1969WIL/ROT		293.1–303.1	2	0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1974PET/TER		298.0–469.2	15	n/a	98.	melpt	*p*	BDCT	1974PET/TER
1982WIL/ING		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986WIL/LAI		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1999ROH/RUZ		304.4–407.1	33	1.00	99.87	chrom	sat	BDCT	1991BAN/GAR
2002LIP/SCH	N	303.1–323.1	2	0.50	99.87	chrom	*p*	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 1998ROH/SCH

Correlated heat capacities (22.35.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1982WIL/ING	298.1	1	0.30		0.159	1.11−2	0.05	1.11−2	1
1986WIL/LAI	298.1	1	1.00	#	0.227	5.32−2	0.23	5.32−2	1
1999ROH/RUZ	304.4–407.1	33	1.00		0.261	6.24−2	0.26	−2.94−2	−13
2002LIP/SCH	303.1–323.1	2	0.50		0.859	1.02−1	0.43	1.02−1	2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1969WIL/ROT	(4.94−1, 2.14, −4.94−1, −1)	1974PET/TER	(9.55−1, 4.34, −1.15−1, 2)

Parameters of regression polynomial (22.35.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	54	37	0.335	6.70−2	0.28	−1.90−2	−9	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.1–407.1		1.791 62+1		1.423 87		1.379 59−1		II

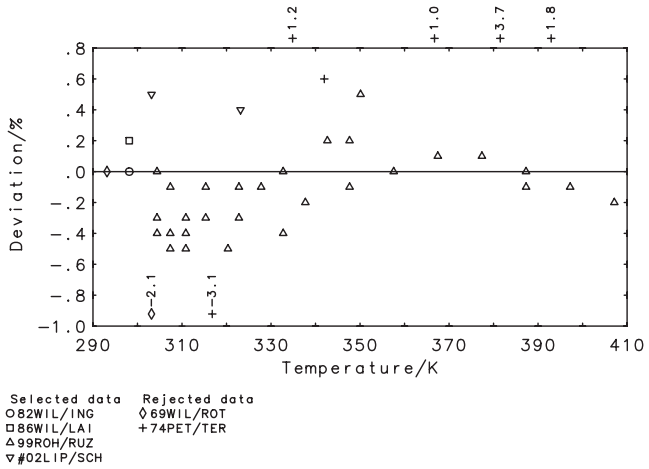

FIG. 39. Deviation plot for 1,2,4-trichlorobenzene (22-035).

Parameters of quasipolynomial equation (22.35.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	54	37	0.339	5.83−2	0.24	−3.40−3	−9

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
298.1–407.1	734.90	2.744 43+3	3.339 89+2	−3.222 67+2	2.544 51+3	4.579 55+2	1.559 03+3	II

Deviation plot for 1,2,4–Trichlorobenzene (22–035) is given in Fig. 39.

6.3.2.9. 1,2-Dichlorobenzene (22-036)

Name:	1,2-Dichlorobenzene
Formula:	$C_6H_4Cl_2$
CAS-RN:	95-50-1
Group No:	22-036

Experimental heat capacities (22.36.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1918NAR		291.1–326.1	4	S	n/a	n/a	n/a	avg	DSIO	1918NAR
1999ROH/RUZ		307.7–377.2	16		1.00	99.98	chrom	sat	BDCT	1991BAN/GAR
2002LIP/SCH	N	263.1–323.1	4		0.50	99.98	chrom	*p*	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 1998ROH/SCH

Correlated heat capacities (22.36.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1999ROH/RUZ	307.7–377.2	16	1.00	0.116	2.45−2	0.12	−1.50−2	−11
2002LIP/SCH	263.1–323.1	4	0.50	0.426	4.40−2	0.21	1.52−2	2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1918NAR	(1.22−1, 0.59, −1.07−1, −4)

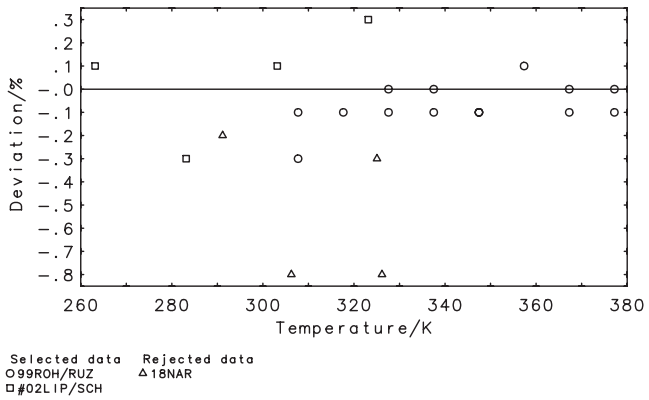

FIG. 40. Deviation plot for 1,2-dichlorobenzene (22-036).

Parameters of regression polynomial (22.36.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	24	20	0.235	3.20−2	0.15	−8.94−3	−9
sat	24	20	0.235	3.20−2	0.15	−8.94−3	−9

T/K	A_1	A_2	A_3	A_4	Uncert.
263.1–377.2	1.710 23+1	−1.256 84−1	4.339 93−1		III
263.1–377.2	1.710 23+1	−1.256 84−1	4.339 93−1		III

Parameters of quasipolynomial equation (22.36.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	24	20	0.246	2.92−2	0.14	7.51−4	−3

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
263.1–377.2	697.30	2.736 86+2	2.661 85+1	−8.326 84	2.510 63+2	7.383 70+1	1.819 45+2	II

Deviation plot for 1,2–Dichlorobenzene (22–036) is given in Fig. 40.

6.3.2.10. 1,3-Dichlorobenzene (22-037)

Name:	1,3-Dichlorobenzene
Formula:	$C_6H_4Cl_2$
CAS-RN:	541-73-1
Group No:	22-037

Experimental heat capacities (22.37.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1918NAR		253.9–327.5	6	S	n/a	n/a	n/a	avg	DSIO	1918NAR
1999ROH/RUZ		308.0–377.6	24		1.00	99.55	chrom	sat	BDCT	1991BAN/GAR
2002LIP/SCH	N	263.1–323.1	4		0.50	99.55	chrom	p	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 1998ROH/SCH

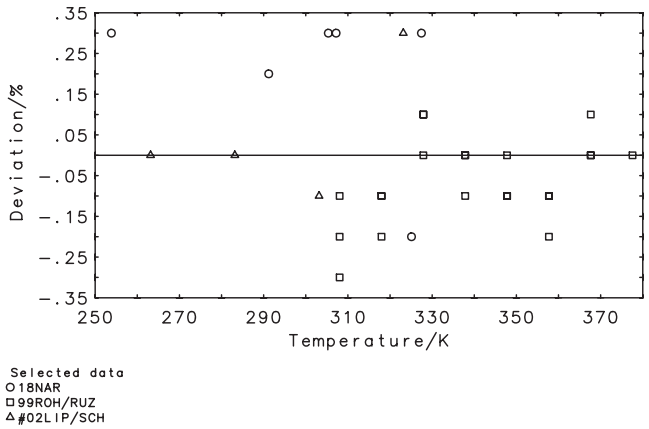

FIG. 41. Deviation plot for 1,3-dichlorobenzene (22-037).

Correlated heat capacities (22.37.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1918NAR	253.9–327.5	6	2.00	#	0.144	5.93−2	0.29	4.44−2	4
1999ROH/RUZ	308.0–377.6	24	1.00		0.110	2.33−2	0.11	−1.19−2	−8
2002LIP/SCH	263.1–323.1	4	0.50		0.323	3.42−2	0.16	1.39−2	0

Parameters of regression polynomial (22.37.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	34	34	0.167	3.60−2	0.17	1.09−3	−4	
T/K		A_1		A_2		A_3	A_4	Uncert.
253.9–377.6		3.625 57+1		−1.810 18+1		5.978 26	−5.652 43−1	III

Parameters of quasipolynomial equation (22.37.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−					
C	34	34	0.292	3.47−2	0.17	6.13−4	−4					
T/K		T_c/K		A_1		A_2	A_3	A_4	A_5	A_6	Uncert.	
253.9–377.6		682.20		7.824 02+2		8.363 40+1	−6.740 97+1	7.389 93+2	1.120 39+2	5.326 41+2	III	

Deviation plot for 1,3–Dichlorobenzene (22–037) is given in Fig. 41.

6.3.2.11. Chlorobenzene (22-039)

Name:	Chlorobenzene
Formula:	C_6H_5Cl
CAS-RN:	108-90-7
Group No:	22-039

Experimental heat capacities (22.39.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		343.8–355.3	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1887SCH		308.6–332.9	6	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1925WIL/DAN	N	293.1–353.1	4	S	n/a	n/a	n/a	p	BSAO	1924WIL/DAN

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1937STU		230.0–320.0	10	S	n/a	n/a	n/a	*p*	BDHO	1937STU
1939PHI		305.5	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1949TSC/RIC3		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1961ROU	N	296.1–318.1	2		n/a	n/a	n/a	*p*	BSAO	1961ROU
1971DES/BHA		298.1–318.1	3	S	n/a	n/a	n/a	*p*	BSIO	1958MUR/VAN
1977FOR/BEN		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1988PER/AIC		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1990RAO/RAJ		318.1–333.1	4		4.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1991TAN/ADA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1992KAL/KOH		293.1–313.1	2		1.00	99.98	chrom	*p*	FSIT	1971PIC/LED
1993SHE		298.1–308.1	2		n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
1994BEN/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994GRO/ROU		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED
1997TAN/NAK		298.1–303.1	2		n/a	***	chrom	*p*	FSIT	1971PIC/LED
1997TAN/TOY		298.1	1		0.01	99.95	chrom	*p*	FSIT	1971PIC/LED
2000TAM/OSA		298.1	1		n/a	99.95	chrom	*p*	FSIO	1985OGA

Reference	Note
1925WIL/DAN	origin of data unclear
1961ROU	constant value in the temperature range 296–318 K obtained by the author

6.3.2.12. 1,6-Dichlorohexane (22-040)

Name:	1,6-Dichlorohexane
Formula:	$C_6H_{12}Cl_2$
CAS-RN:	2163-00-0
Group No:	22-040

Experimental heat capacities (22.40.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1985LAI/GRO		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
2003GOR/TKA		284.2–353.1	30	0.15	99.5	chrom	*p*	BDCT	2000ERN/CHO
2004GON/PEL		283.1–323.1	9	n/a	99.5	chrom	*p*	BDCT	1970PAZ/PAZ

Correlated heat capacities (22.40.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1985LAI/GRO	298.1	1	0.50	#	0.650	9.36−2	0.32	−9.36−2	−1
2003GOR/TKA	284.2–353.1	30	0.15		0.303	1.36−2	0.05	−3.60−4	7
2004GON/PEL	283.1–323.1	9	0.50	#	0.186	2.68−2	0.09	2.43−2	9

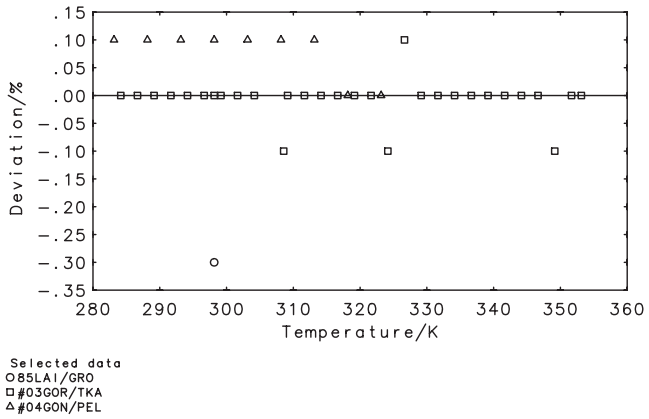

FIG. 42. Deviation plot for 1,6-dichlorohexane (22-040).

Parameters of regression polynomial (22.40.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	40	40	0.307	2.37−2	0.08	2.86−3	15

T/K	A_1	A_2	A_3	A_4	Uncert.
283.1–353.1	2.457 99+1	−4.735 66−1	6.456 32−1		III

Deviation plot for 1,6–Dichlorohexane (22–040) is given in Fig. 42.

6.3.2.13. 1-Chloropentane (22-054)

Name:	1-Chloropentane
Formula:	$C_5H_{11}Cl$
CAS-RN:	543-59-9
Group No:	22-054

Experimental heat capacities (22.54.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.54.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	0.50	#	0.356	4.01−2	0.18	−3.16−2	−2
2005CHO/GOR	284.1–353.1	29	0.50	#	0.153	1.81−2	0.08	2.22−3	9

Parameters of regression polynomial (22.54.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	31	31	0.182	2.13−2	0.09	3.42−5	7

T/K	A_1	A_2	A_3	A_4	Uncert.
284.1–353.1	1.776 71+1	8.128 72−2	5.199 43−1		II

Deviation plot for 1–Chloropentane (22–054) is given in Fig. 43.

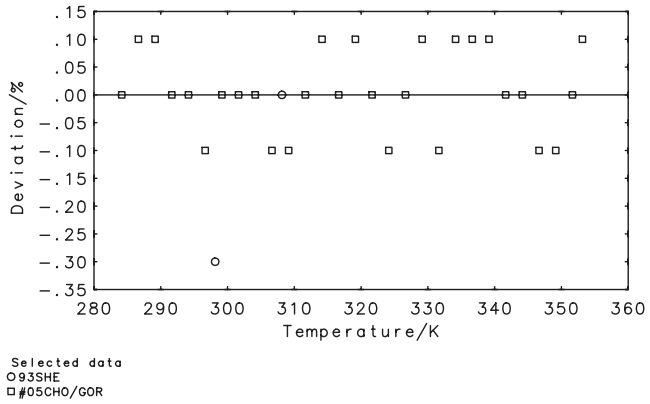

FIG. 43. Deviation plot for 1-chloropentane (22-054).

6.3.2.14. 1-Chlorohexane (22-060)

Name:	1-Chlorohexane
Formula:	$C_6H_{13}Cl$
CAS-RN:	544-10-5
Group No:	22-060

Experimental heat capacities (22.60.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2004BOL/NER		293.1–373.1	17	3.00	99.3	chrom	p	BDCT	2004BOL/NER
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.60.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.204	5.34−2	0.20	−4.48−3	0
2005CHO/GOR	284.1–353.1	29	0.15		0.890	3.67−2	0.13	1.04−4	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2004BOL/NER	(1.56, 6.13, −1.56, −13)

Parameters of regression polynomial (22.60.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	48	31	0.908	3.99−2	0.15	−1.91−4	−4	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–353.1		1.756 46+1		1.864 74		3.303 07−1		IV

Deviation plot for 1–Chlorohexane (22–060) is given in Fig. 44.

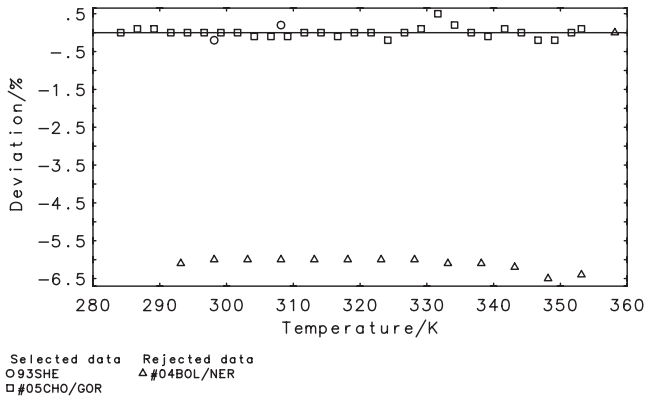

FIG. 44. Deviation plot for 1-chlorohexane (22-060).

6.3.2.15. 1-Chloroheptane (22-062)

Name:	1-Chloroheptane
Formula:	$C_7H_{15}Cl$
CAS-RN:	629-06-1
Group No:	22-062

Experimental heat capacities (22.62.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (22.62.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.199	5.94−2	0.20	1.79−2	0
2005CHO/GOR	284.1–353.1	29	0.15		0.565	2.64−2	0.08	1.77−5	4

Parameters of regression polynomial (22.62.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	31	31	0.577	3.12−2	0.10	1.17−3	4

T/K	A_1	A_2	A_3	A_4	Uncert.
284.1–353.1	2.131 72+1	1.295 27	4.921 06−1		IV

Deviation plot for 1–Chloroheptane (22–062) is given in Fig. 45.

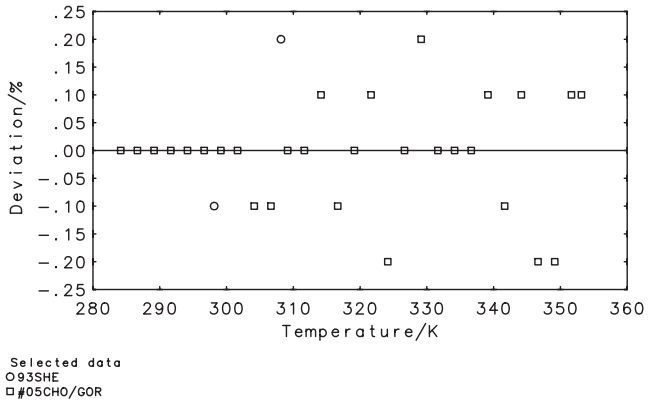

FIG. 45. Deviation plot for 1-chloroheptane (22-062).

6.3.2.16. 1-Chlorooctane (22-063)

Name:	1-Chlorooctane
Formula:	$C_8H_{17}Cl$
CAS-RN:	111-85-3
Group No:	22-063

Experimental heat capacities (22.63.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	*p*	BDCT	2000ERN/CHO

Correlated heat capacities (22.63.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.137	4.52−2	0.14	−2.08−2	0
2005CHO/GOR	284.1–353.1	29	0.15		0.727	3.78−2	0.11	1.16−4	−1

Parameters of regression polynomial (22.63.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	31	31	0.740	4.04−2	0.12	−1.23−3	−1	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–353.1		2.154 10+1		2.935 18		3.158 22−1		III

Deviation plot for 1-Chlorooctane (22–063) is given in Fig. 46.

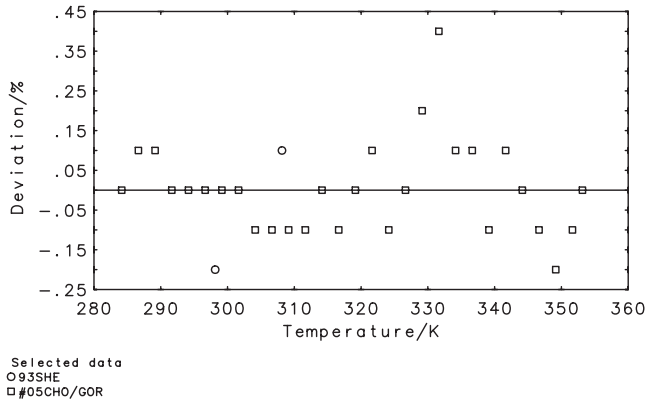

FIG. 46. Deviation plot for 1-chlorooctane (22-063).

6.3.2.17. 1-Chloro-4-methylbenzene (22-065)

Name:	1-Chloro-4-methylbenzene
Formula:	C_7H_7Cl
CAS-RN:	106-43-4
Group No:	22-065

Experimental heat capacities (22.65.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996VAN/ALV		283.8–304.9	10	0.20	99.73	melpt	p	BSAO	1987VAN/VAN

Parameters of regression polynomial (22.65.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	10	10	0.115	4.82−3	0.02	2.29−6	−1	
T/K		A_1		A_2		A_3	A_4	Uncert.
283.8–304.9		2.997 53+1		−9.182 15		2.097 46		II

6.3.2.18. 1-Chlorononane (22-066)

Name:	1-Chlorononane
Formula:	$C_9H_{19}Cl$
CAS-RN:	2473-01-0
Group No:	22-066

Experimental heat capacities (22.66.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004BOL/NER		293.1–373.1	17	3.00	98.4	chrom	p	BDCT	2004BOL/NER

Parameters of regression polynomial (22.66.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	17	17	0.016	1.84−2	0.05	3.25−5	−2	
T/K		A_1		A_2		A_3	A_4	Uncert.
293.1–373.1		1.979 87+1		5.310 99				V

6.3.2.19. 1-Chlorodecane (22-067)

Name:	1-Chlorodecane
Formula:	$C_{10}H_{21}Cl$
CAS-RN:	1002-69-3
Group No:	22-067

Experimental heat capacities (22.67.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	*p*	BDCT	2000ERN/CHO

Correlated heat capacities (22.67.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002GOR/WAS	298.1	1	0.20	0.495	3.99−2	0.10	3.99−2	1
2005CHO/GOR	284.1–353.1	29	0.15	0.465	2.95−2	0.07	−7.32−4	3

Parameters of regression polynomial (22.67.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	30	30	0.491	3.15−2	0.07	6.24−4	4	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–53.1		3.089 69+1		7.583 72−1		8.016 01−1		II

Deviation plot for 1–Chlorodecane (22–067) is given in Fig. 47.

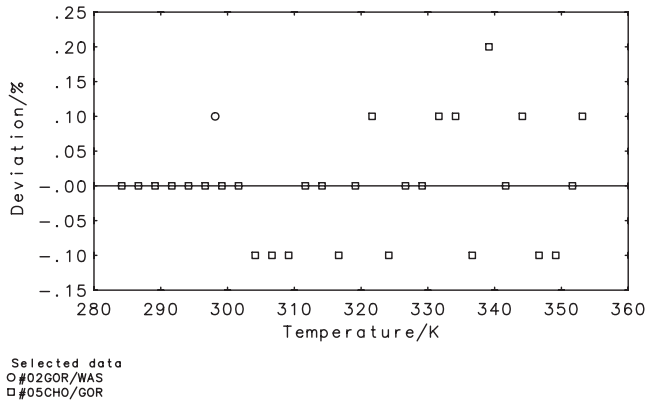

FIG. 47. Deviation plot for 1-chlorodecane (22-067).

6.3.2.20. 1-Chlorohexadecane (22-068)

Name:	1-Chlorohexadecane
Formula:	$C_{16}H_{33}Cl$
CAS-RN:	4860-03-1
Group No:	22-068

Experimental heat capacities (22.68.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002GOR/WAS		298.15	2.00	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

6.3.3. Subgroup 23: brominated hydrocarbons

6.3.3.1. 1,2-Dibromoethane (23-017)

Name:	1,2-Dibromoethane
Formula:	$C_2H_4Br_2$
CAS-RN:	106-93-4
Group No:	23-017

Experimental heat capacities (23.17.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1933LEB/MOE		283.3–298.5	5	n/a	n/a	n/a	*p*	BSIO	1933LEB/MOE
1939RAI	N	283.3–321.7	9	2.00	99.92	melpt	*p*	BDHO	1937STU
1940PIT1		286.5–318.0	4	0.20	99.74	melpt	*p*	BSIO	1928LAT/GRE
1948KUR		309.1–345.7	3	n/a	n/a	n/a	avg	DSIO	1947KUR
1949DHO/JUN		293.1	1	n/a	n/a	n/a	*p*	BDHO	1949WUY/JUN
1949TSC/RIC3		298.1	1	n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1949WUY/JUN		310.1	1	n/a	n/a	n/a	*p*	BDHO	1949WUY/JUN
1965FIN/GRU		300.0	1	0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1969WIL/SCH		293.1–313.1	3	0.40	n/a	n/a	*p*	BDAO	1965FIN/GRU
1993SHE		298.1–308.1	2	n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
1995LAI/LOP		298.1	1	n/a	99.9	chrom	*p*	FSIT	1971PIC/LED
2000ERN/CHO		291.8–327.1	8	0.10	99.0	anal	*p*	BDCT	2000ERN/CHO

Reference	Notes
1939RAI	data from a graph only

Correlated heat capacities (23.17.2)

Reference	*T*/K	nPts	$\sigma_r C$/%		d_w	*d*/R	d_r/%	d_b/R	+/−
1940PIT1	286.5–318.0	4	1.00	#	0.363	5.96−2	0.36	−4.68−2	−4
1949TSC/RIC3	298.1	1	3.00	#	0.270	1.32−1	0.81	−1.32−1	−1
1965FIN/GRU3	300.0	1	1.00	#	0.817	1.33−1	0.82	−1.33−1	−1
1993SHE	308.1	1	1.00	#	0.326	5.34−2	0.33	−5.34−2	−1
2000ERN/CHO	291.8–327.1	8	0.50	#	0.211	1.74−2	0.11	1.23−2	4

Rejected data: Reference (*d*/R, d_r, d_b/R, +/-)

1933LEB/MOE	(1.29−1, 0.80, −9.95−2, −1)	1939RAI	(3.31−1, 2.06, −2.94−1, −8)
1948KUR	(5.52−2, 0.33, 5.52−2, 1)	1949DHO/JUN	(1.44−1, 0.89, −1.44−1, −1)
1949WUY/JUN	(2.34−1, 1.44, −2.34−1, −1)	1969WIL/SCH	(1.83−1, 1.13, −1.81−1, −3)
1995LAI/LOP	(6.97−2, 0.42, 6.97−2, 1)		

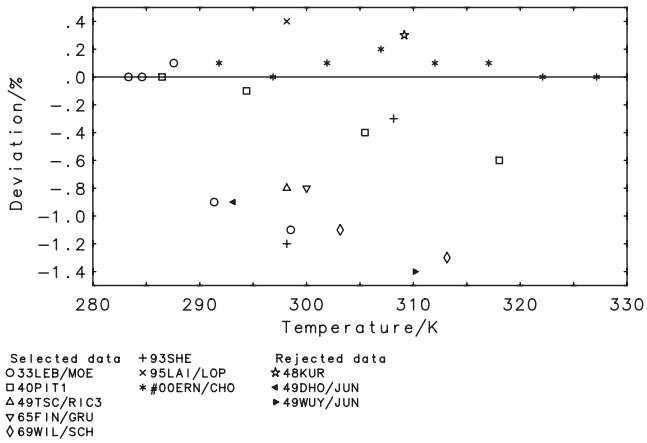

FIG. 48. Deviation plot for 1,2-dibromoethane (23-017).

Parameters of regression polynomial (23.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	39	15	0.379	6.74−2	0.41	−2.71−2	−3	
T/K		A_1		A_2		A_3	A_4	Uncert.
286.5–327.1		1.897 37+1		−2.464 23		5.360 84−1		IV

Deviation plot for 1,2–Dibromoethane (23–017) is given in Fig. 48.

6.3.3.2. Bromoethane (23-018)

Name:	Bromoethane
Formula:	C_2H_5Br
CAS-RN:	74-96-4
Group No:	23-018

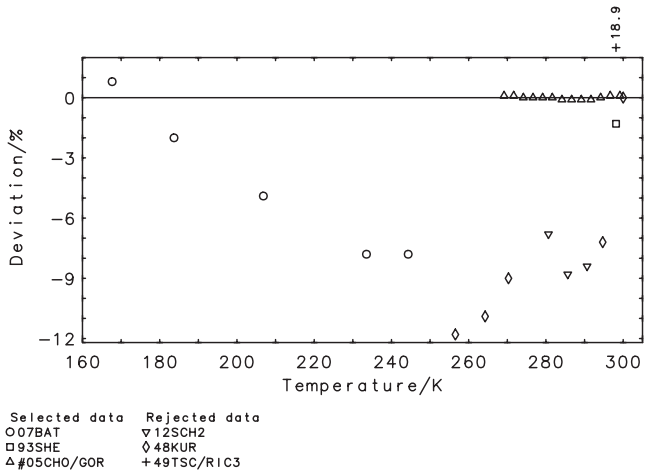

FIG. 49. Deviation plot for bromoethane (23-018).

Experimental heat capacities (23.18.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1907BAT	N	167.7–244.3	5	n/a	n/a	n/a	p	BSIO	1907BAT
1912SCH2		280.6–290.6	3	n/a	n/a	n/a	p	BSIO	1912SCH1
1948KUR		256.5–300.0	5	n/a	n/a	n/a	avg	DSIO	1947KUR
1949TSC/RIC3		298.1	1	n/a	n/a	n/a	p	BSIO	1949TSC/RIC1
1993SHE		298.1	1	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		269.1–299.1	13	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Reference	Notes
1907BAT	same data in 1908BAT

Correlated heat capacities (23.18.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1907BAT	167.7–233.5	4	5.00	#	0.945	5.20−1	4.72	−3.81−1	−2
1993SHE	298.1	1	1.00	#	1.289	1.64−1	1.29	−1.64−1	−1
2005CHO/GOR	269.1–299.1	13	0.15		0.470	9.01−3	0.07	4.23−4	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1912SCH2	(9.45−1, 8.02, −9.39−1, −3)	1948KUR	(1.12, 9.88, −1.10, −4)
1949TSC/RIC3	(3.01, 18.95, 3.01, 1)		

Parameters of regression polynomial (23.18.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	28	18	0.735	2.72−1	2.46	−9.36−2	−5	
T/K		A_1		A_2		A_3	A_4	Uncert.
167.7–299.1		5.539 70		3.736 66		−4.265 50−1		IV

Deviation plot for Bromoethane (23–018) is given in Fig. 49.

6.3.3.3. 1,3-Dibromopropane (23-022)

Name:	1,3-Dibromopropane
Formula:	$C_3H_6Br_2$
CAS-RN:	109-64-8
Group No:	23-022

Experimental heat capacities (23.22.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1948KUR		332.3–358.3	3	n/a	n/a	n/a	avg	DSIO	1947KUR
1950CRO/SMY2		243.1–245.6	2	1.40	n/a	n/a	p	BDHO	1950KUS/CRO
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2000ERN/CHO		291.8–327.1	8	0.10	98.0	anal	p	BDCT	2000ERN/CHO

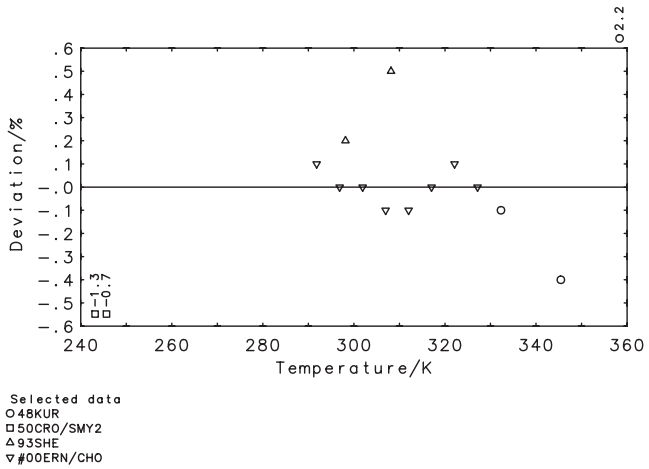

FIG. 50. Deviation plot for 1,3-dibromopropane (23-022).

Correlated heat capacities (23.22.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1948KUR	332.3–358.4	3	5.00	#	0.255	2.69−1	1.27	1.23−1	−1
1950CRO/SMY2	243.1–245.6	2	1.40		0.739	1.93−1	1.03	−1.84−1	−2
1993SHE	298.1–308.1	2	1.00	#	0.423	8.40−2	0.42	7.85−2	2
2000ERN/CHO	291.8–327.1	8	0.10		0.668	1.32−2	0.07	4.43−5	3

Parameters of regression polynomial (23.22.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	15	15	0.659	1.60−1	0.79	1.07−2	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
243.1–358.4		1.709 68+1		1.641 27−1		2.310 48−1		IV

Deviation plot for 1,3–Dibromopropane (23–022) is given in Fig. 50.

6.3.3.4. 1-Bromopropane (23-023)

Name:	1-Bromopropane
Formula:	C_3H_7Br
CAS-RN:	106-94-5
Group No:	23-023

Experimental heat capacities (23.23.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		305.1–323.3	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1948KUR		268.1–312.9	3		n/a	n/a	n/a	avg	DSIO	1947KUR
1949TSC/RIC3		298.1	1		n/a	n/a	n/a	p	BSIO	1949TSC/RIC1
1993SHE		298.1–308.1	2		n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		269.1–326.6	24		0.15	99.0	chrom	p	BDCT	2000ERN/CHO

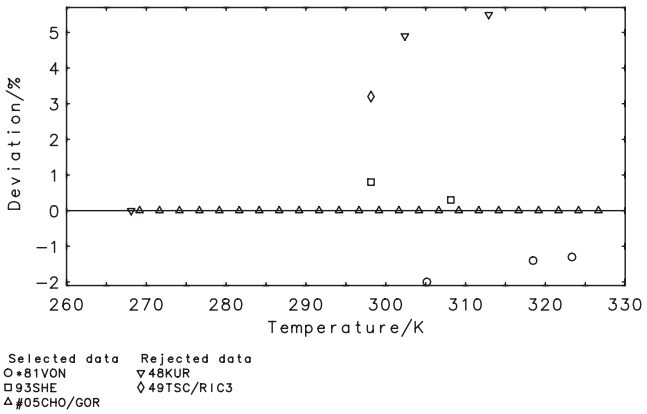

FIG. 51. Deviation plot for 1-bromopropane (23-023).

Correlated heat capacities (23.23.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1881VON	305.1–323.3	3	3.00	#	0.536	2.59−1	1.61	−2.55−1	−3
1993SHE	298.1–308.1	2	1.00	#	0.633	1.02−1	0.63	9.34−2	2
2005CHO/GOR	269.1–326.6	24	0.15		0.141	3.38−3	0.02	−8.90−5	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1948KUR	(8.98−1, 5.23, 8.95−1, 2)	1949TSC/RIC3	(5.34−1, 3.22, 5.34−1, 1)

Parameters of regression polynomial (23.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	33	29	0.287	9.24−2	0.57	−2.00−2	−1	
T/K		A_1		A_2		A_3	A_4	Uncert.
269.1–326.6		1.494 04+1		−1.246 66		5.432 94−1		III

Deviation plot for 1–Bromopropane (23–023) is given in Fig. 51.

6.3.3.5. 1-Bromobutane (23-025)

Name:	1-Bromobutane
Formula:	C_4H_9Br
CAS-RN:	109-65-9
Group No:	23-025

Experimental heat capacities (23.25.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931DEE		176.9–292.3	27	n/a	n/a	n/a	p	BDAO	1931DEE
1948KUR		307.6–331.1	2	n/a	n/a	n/a	avg	DSIO	1947KUR
1949TSC/RIC3		298.1	1	n/a	n/a	n/a	p	BSIO	1949TSC/RIC1
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

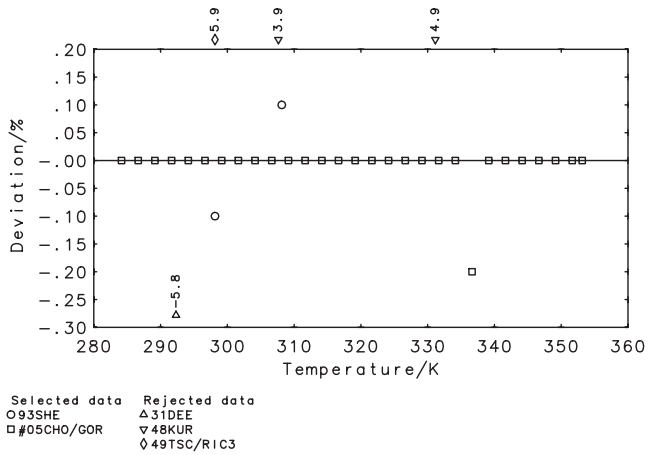

FIG. 52. Deviation plot for 1-bromobutane (23-025).

Correlated heat capacities (23.25.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.129	2.55−2	0.13	3.75−3	0
2005CHO/GOR	284.1–353.1	29	0.15		0.246	7.59−3	0.04	−5.92−7	9
	Rejected data: Reference (d/R, d_r, d_b/R, +/−)								
1931DEE	(1.06, 5.78, −1.06, −1)		1948KUR			(9.40−1, 4.45, 9.32−1, 2)			
1949TSC/RIC3	(1.23, 5.90, 1.23, 1)								

Parameters of regression polynomial (23.25.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	61	31	0.253	1.03−2	0.05	2.41−4	9	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–353.1		1.689 27+1		−7.977 60−1		5.642 08−1		III

Deviation plot for 1–Bromobutane (23–025) is given in Fig. 52.

6.3.3.6. 1-Bromopentane (23-030)

Name:	1-Bromopentane
Formula:	$C_5H_{11}Br$
CAS-RN:	110-53-2
Group No:	23-030

Experimental heat capacities (23.30.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931DEE		195.8–290.7	10	n/a	n/a	n/a	p	BDAO	1931DEE
1950KUS/CRO		190.1–206.6	6	1.50	n/a	n/a	p	BDHO	1950KUS/CRO
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

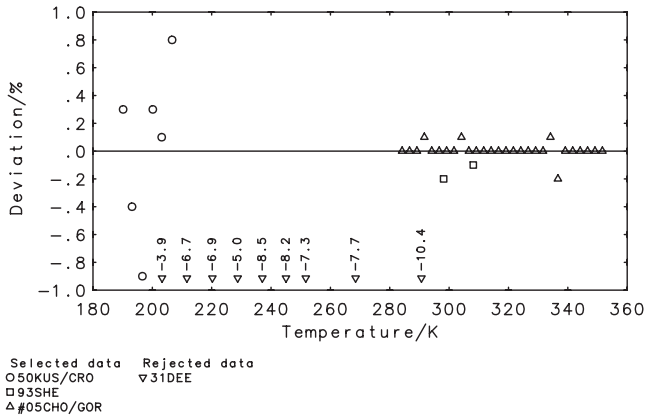

FIG. 53. Deviation plot for 1-bromopentane (23-030).

Correlated heat capacities (23.30.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1950KUS/CRO	190.1–206.6	6	1.50		0.361	1.12−1	0.54	1.43−2	2
1993SHE	298.1–308.1	2	1.00	#	0.138	3.18−2	0.14	−2.91−2	−2
2005CHO/GOR	284.1–353.1	29	0.15		0.344	1.24−2	0.05	3.03−5	2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1931DEE	(1.45, 7.22, −1.40, −10)

Parameters of regression polynomial (23.30.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	47	37	0.353	4.91−2	0.23	7.62−4	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
190.1–353.1		2.065 03+1		−1.450 65		7.524 47−1		III

Deviation plot for 1–Bromopentane (23–030) is given in Fig. 53.

6.3.3.7. 1-Bromohexane (23-034)

Name:	1-Bromohexane
Formula:	$C_6H_{13}Br$
CAS-RN:	111-25-1
Group No:	23-034

Experimental heat capacities (23.34.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1931DEE		214.0–289.8	12	n/a	n/a	n/a	p	BDAO	1931DEE
1949TSC/RIC3		298.1	1	n/a	n/a	n/a	p	BSIO	1949TSC/RIC1
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

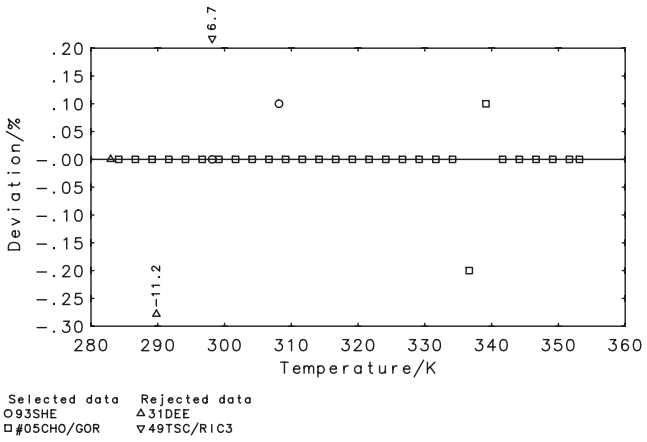

FIG. 54. Deviation plot for 1-bromohexane (23-034).

Correlated heat capacities (23.34.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.064	1.71−2	0.06	1.42−2	2
2005CHO/GOR	284.1–353.1	29	0.15		0.329	1.37−2	0.05	−7.89−6	5

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1931DEE	(2.63, 11.22, −2.63, −1)	1949TSC/RIC3	(1.91, 6.73, 1.91, 1)

Parameters of regression polynomial (23.34.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	44	31	0.335	1.47−2	0.05	9.10−4	7	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–353.1		2.238 95+1		−8.823 32−1		7.492 36−1		III

Deviation plot for 1–Bromohexane (23–034) is given in Fig. 54.

6.3.3.8. 1-Bromoheptane (23-036)

Name:	1-Bromoheptane
Formula:	$C_7H_{15}Br$
CAS-RN:	629-04-9
Group No:	23-036

Experimental heat capacities (23.36.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1950CRO/SMY1		222.1–231.1	4	1.00	n/a	n/a	p	BDHO	1950KUS/CRO
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (23.36.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	0.50	#	0.983	1.47−1	0.49	−1.42−1	−2
2005CHO/GOR	284.1–353.1	29	0.15		0.306	1.44−2	0.05	9.04−4	9

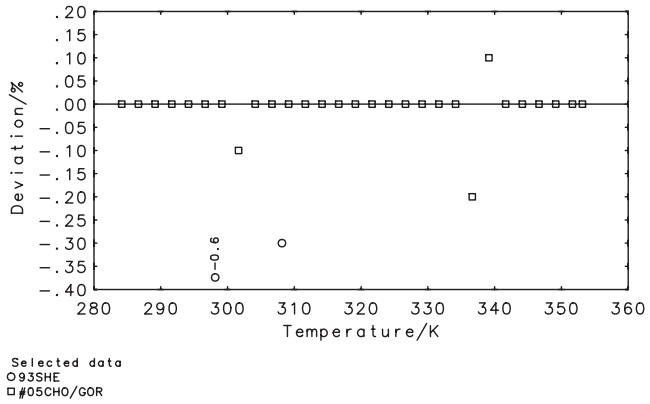

FIG. 55. Deviation plot for 1-bromoheptane (23-036).

Parameters of regression polynomial (23.36.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	35	31	0.407	4.20−2	0.14	−8.33−3	7

T/K	A_1	A_2	A_3	A_4	Uncert.
284.1–353.1	2.465 97+1	−5.221 05−1	7.753 44−1		II

Deviation plot for 1–Bromoheptane (23–036) is given in Fig. 55.

6.3.3.9. 1-Bromononane (23-038)

Name:	1-Bromononane
Formula:	$C_9H_{19}Br$
CAS-RN:	693-58-3
Group No:	23-038

Experimental heat capacities (23.38.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1950CRO/SMY1		248.6–257.1	4	1.00	n/a	n/a	p	BDHO	1950KUS/CRO
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (23.38.2)

Reference	T/K	nPts	$\sigma_r C/\%$		d_w	d/R	$d_r/\%$	d_b/R	+/−
1950CRO/SMY1	248.6–257.1	4	2.00	#	0.648	4.47−1	1.29	−3.90−1	−4
2005CHO/GOR	284.1–353.1	29	0.15		0.286	1.67−2	0.04	3.25−4	6

Parameters of regression polynomial (23.38.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	33	33	0.367	1.64−1	0.47	−4.69−2	2

T/K	A_1	A_2	A_3	A_4	Uncert.
248.6–353.1	2.925 30+1	1.488 50−1	8.306 11−1		II

Deviation plot for 1–Bromononane (23–038) is given in Fig. 56.

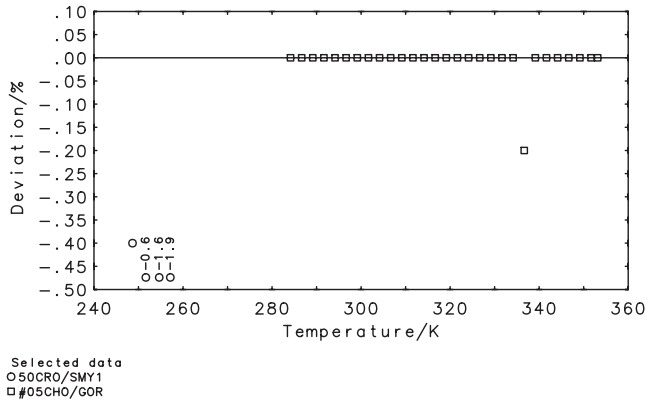

FIG. 56. Deviation plot for 1-bromononane (23-038).

6.3.3.10. 1,4-Dibromobutane (23-041)

Name:	1,4-Dibromobutane
Formula:	$C_4H_8Br_2$
CAS-RN:	110-52-1
Group No:	23-041

Experimental heat capacities (23.41.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
2000ERN/CHO		291.8-327.1	8	0.10	99.0	anal	*p*	BDCT	2000ERN/CHO

Correlated heat capacities (23.41.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	3.00	#	0.123	8.61−2	0.37	5.70−2	0
2000ERN/CHO	291.8–327.1	8	0.10		1.368	3.21−2	0.14	7.22−5	2

Parameters of regression polynomial (23.41.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	10	10	1.464	5.74−2	0.25	1.15−2	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
291.8–327.1		3.752 64+1		−1.136 07+1		2.176 67		V

Deviation plot for 1,3–Dibromobutane (23–041) is given in Fig. 57.

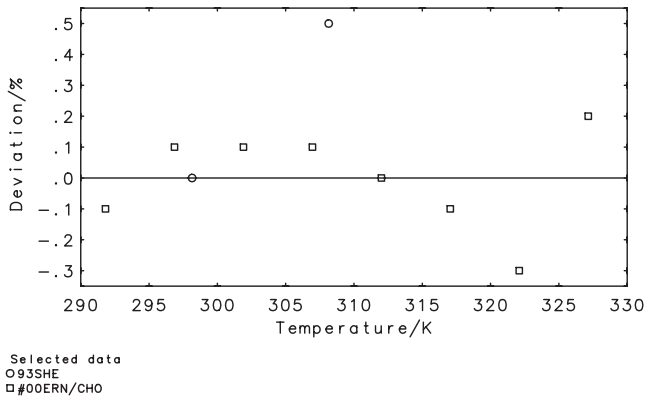

FIG. 57. Deviation plot for 1,4-dibromobutane (23-041).

6.3.3.11. 1,5-Dibromopentane (23-044)

Name:	1,5-Dibromopentane
Formula:	$C_5H_{10}Br_2$
CAS-RN:	111-24-0
Group No:	23-044

Experimental heat capacities (23.44.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000ERN/CHO		291.8–327.1	8	0.10	97.0	anal	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (23.44.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	8	8	1.559	4.17−2	0.16	8.18−5	−2	
T/K		A_1		A_2		A_3	A_4	Uncert.
291.8–327.1		2.889 12+1		−4.036 30		1.087 45		IV

6.3.3.12. 1,6-Dibromohexane (23-045)

Name:	1,6-Dibromohexane
Formula:	$C_6H_{12}Br_2$
CAS-RN:	629-03-8
Group No:	23-045

Experimental heat capacities (23.45.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000ERN/CHO		291.8–327.1	8	0.10	97.0	anal	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (23.45.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	8	8	2.015	6.05−2	0.20	1.53−4	0

T/K	A_1	A_2	A_3	A_4	Uncert.
291.8–327.1	2.126 34+1	2.576 48	1.011 94−1		IV

6.3.3.13. 1-Bromo-4-methylbenzene (23-046)

Name:	1-Bromo-4-methylbenzene
Formula:	C_7H_7Br
CAS-RN:	106-38-7
Group No:	23-046

Experimental heat capacities (23.46.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996VAN/ALV		305.8–330.4	9	0.20	99.994	melpt	p	BSAO	1987VAN/VAN

Parameters of regression polynomial (23.46.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	9	9	0.123	5.49−3	0.02	2.54−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
305.8–330.4	1.569 84+1	1.030 40	3.240 74−1		I

6.3.3.14. 1-Bromotricyclo[3.3.1.1^{3,7}]decane (23-047)

Name:	1-Bromotricyclo[3.3.1.1^{3,7}]decane
Formula:	$C_{10}H_{15}Br$
CAS-RN:	768-90-1
Group No:	23-047

Experimental heat capacities (23.47.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004BLO/KAB		391.8–430.0	3	S	2.00	99.84	chrom	p	BDHT	1992KAB/KOZ
2005BAZ/BLO	N	391.8–430.0	5	S	2.00	99.95	chrom	p	BDHT	1992KAB/KOZ

Correlated heat capacities (23.47.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004BLO/KAB	391.8–430.0	3	2.00	0.004	3.37−3	0.01	1.48−3	1
2005BAZ/BLO	391.8–430.0	5	2.00	0.003	2.43−3	0.01	−8.90−4	−1

Parameters of regression polynomial (23.47.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	8	8	0.005	3.56−3	0.01	−9.54−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
391.8–430.0	3.872 67+1	−9.895 66−1	1.694 31−1		IV

Deviation plot for 1-Bromotricyclo[3.3.1.1^{3,7}]decane (23-047) is given in Fig. 58.

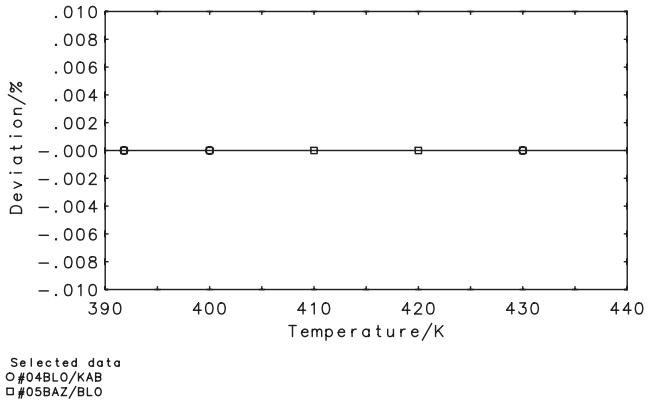

FIG. 58. Deviation plot for 1-bromotricyclo[3.3.1.1^{3,7}]decane (23-047).

6.3.3.15. 1-Bromodecane (23-048)

Name:	1-Bromodecane
Formula:	$C_{10}H_{21}Br$
CAS-RN:	112-29-8
Group No:	23-048

Experimental heat capacities (23.48.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CHO/GOR		284.1–353.1	29	0.15	99.0	chrom	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (23.48.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	29	29	0.303	1.93−2	0.05	1.58−5	7	
T/K		A_1		A_2		A_3	A_4	Uncert.
284.1–353.1		3.689 75+1		−2.842 30		1.386 56		II

6.3.4. Sub group 24: iodinated hydrocarbons

6.3.4.1. 1-Iodohexane (24-015)

Name:	1-Iodohexane
Formula:	$C_6H_{13}I$
CAS-RN:	638-45-9
Group No:	24-015

Experimental heat capacities (24.15.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2004BOL/NER		293.1-373.1	17	3.00	99.4	chrom	p	BDCT	2004BOL/NER

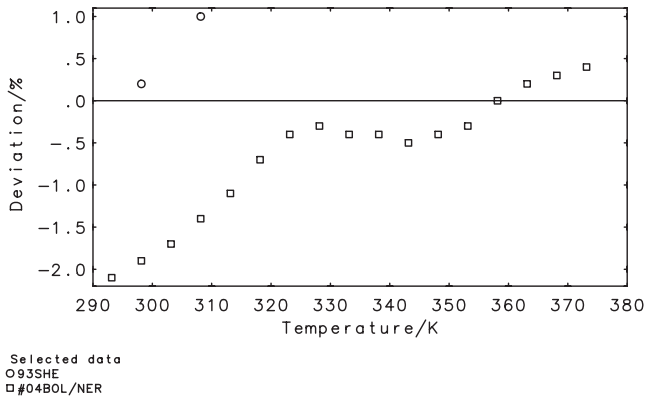

FIG. 59. Deviation plot for 1-iodohexane (24-015).

Correlated heat capacities (24.15.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.717	1.95−1	0.72	1.65−1	2
2004BOL/NER	293.1–373.1	17	3.00		0.322	2.56−1	0.97	−1.67−1	−11

Parameters of regression polynomial (24.15.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	19	19	0.418	2.73−1	1.03	−1.32−1	−9	
T/K		A_1		A_2		A_3	A_4	Uncert.
293.1–373.1		2.397 59+1		−3.965 22−1		4.392 70−1		V

Deviation plot for 1–Iodohexane (24–015) is given in Fig. 59.

6.3.4.2. 1-Iodoheptane (24-016)

Name:	1-Iodoheptane
Formula:	$C_7H_{15}I$
CAS-RN:	4282-40-0
Group No:	24-016

Experimental heat capacities (24.16.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993SHE		298.1–308.1	2	n/a	99.9	chrom	p	DDCT	1971KON/SUU
2004BOL/NER		293.1–373.1	17	3.00	98.8	chrom	p	BDCT	2004BOL/NER

Correlated heat capacities (24.16.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993SHE	298.1–308.1	2	1.00	#	0.240	7.38−2	0.24	6.71−2	2
2004BOL/NER	293.1–373.1	17	3.00		0.125	1.14−1	0.38	−6.98−2	−11

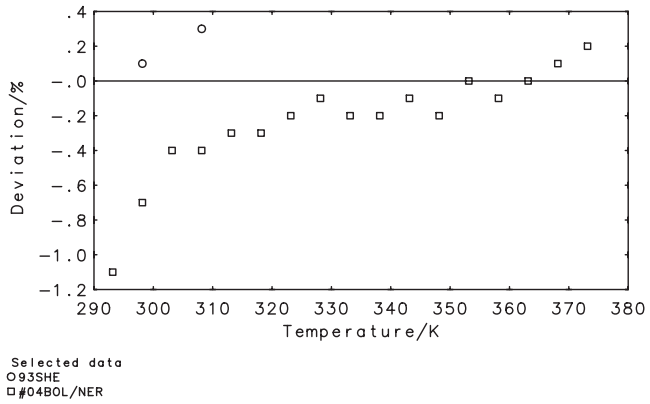

FIG. 60. Deviation plot for 1-iodoheptane (24-016).

Parameters of regression polynomial (24.16.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.155	1.20−1	0.40	−5.54−2	−9

T/K	A_1	A_2	A_3	A_4	Uncert.
293.1–373.1	9.491 81	9.405 54	−8.196 52−1		V

Deviation plot for 1–Iodoheptane (24–016) is given in Fig. 60.

6.3.4.3. 1,4-Diiodobenzene (24-017)

Name:	1,4-Diiodobenzene
Formula:	$C_6H_4I_2$
CAS-RN:	624-38-4
Group No:	24-017

Experimental heat capacities (24.17.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001VAN/OON1		405.9–411.3	5	0.20	n/a	n/a	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (24.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.524	2.62−2	0.10	3.66−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
405.9–411.3	8.672 50+2	−4.144 97+2	5.099 74+1		III

6.3.4.4. 1-Iodo-4-methylbenzene (24-018)

Name:	1-Iodo-4-methylbenzene
Formula:	C_7H_7I
CAS-RN:	624-31-7
Group No:	24-018

Experimental heat capacities (24.18.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996VAN/ALV		309.9–331.3	12	0.20	99.7	chrom	p	BSAO	1987VAN/VAN

Parameters of regression polynomial (24.18.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	11	1.103	5.01−2	0.22	1.54−4	3

T/K	A_1	A_2	A_3	A_4	Uncert.
309.9–328.2	8.827 84+1	−4.421 90+1	7.426 04		III

6.3.5. Subgroup 25: mixed halogenated hydrocarbons

6.3.5.1. 2-Chloro-1,1,1,2-tetrafluoroethane (25-036)

Name:	2-Chloro-1,1,1,2-tetrafluoroethane
Formula:	C_2HClF_4
CAS-RN:	2837-89-0
Group No:	25-036

Experimental heat capacities (25.36.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993DU/SUV2	N	216.6–261.1	11	S	n/a	n/a	n/a	p	n/a	n/a
2000MAG		94.3–317.9	116		0.70	99.9985	anal	sat	BSAO	1961GOO

Reference	Notes
1993DU/SUV2	table is based on experimental data from the database at the National Institute of Standards and Technology (NIST)

Correlated heat capacities (25.36.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1993DU/SUV2	216.6–261.1	11	5.00	#	0.737	6.36−1	3.68	−1.56−1	−5
2000MAG	94.3–317.9	116	0.70		0.364	4.51−2	0.25	6.48−4	−8

Parameters of regression polynomial (25.36.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	127	127	0.415	1.94−1	1.13	−1.29−2	−13
sat	127	127	0.378	1.90−1	1.10	−1.16−2	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
94.3–317.9	1.644 42+1	−2.081 43	9.385 72−1		III
94.3–317.9	1.622 60+1	−1.810 62	8.597 11−1		II

Deviation plot for 2–Chloro—1,1,1,2–tetrafluoroethane (25–036) is given in Fig. 61.

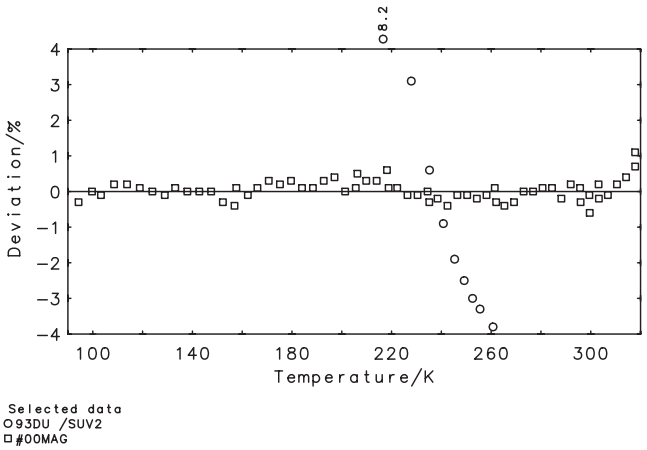

FIG. 61. Deviation plot for 2-chloro-1,1,1,2-tetrafluoroethane (25-036).

6.3.5.2. 2,2-Dichloro-1,1,1-trifluoroethane (25-038)

Name:	2,2-Dichloro-1,1,1-trifluoroethane
Formula:	$C_2HCl_2F_3$
CAS-RN:	306-83-2
Group No:	25-038

Experimental heat capacities (25.38.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991DU/SUV		298.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1991NAK		275.6–300.0	4		0.40	99.82	anal	*p*	FSAO	1989SAI/SAT
1993DU/SUV1	N	249.5–301.0	11	S	n/a	n/a	n/a	*p*	n/a	n/a
2000MAG		166.9–304.1	88		0.70	99.99	anal	sat	BSAO	1961GOO
2002VAR/DRU		146.4–297.5	103		0.30	99.99	melpt	*p*	BSAO	1997VAR/DRU1

Reference	Notes
1993DU/SUV1	table is based on experimental data from the database at the National Institute of Standards and Technology

Correlated heat capacities (25.38.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2000MAG	166.9–304.1	88	0.70		0.482	6.14−2	0.34	3.10−2	39
2002VAR/DRU	146.4–297.5	103	0.70	#	0.458	5.77−2	0.32	−2.57−2	−37

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1991DU/SUV	(1.57−3, 0.01, −1.57−3, 0)	1991NAK	(3.38−1, 1.80, 3.38−1, 4)
1993DU/SUV1	(1.63, 10.56, −1.36, −11)		

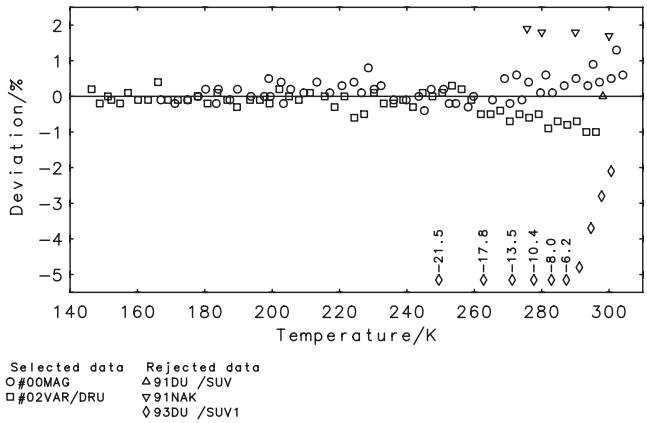

FIG. 62. Deviation plot for 2,2-dichloro-1,1,1-trifluoroethane (25-038).

Parameters of regression polynomial (25.38.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	207	191	0.473	5.99−2	0.33	3.94−4	2
sat	207	191	0.470	5.95−2	0.33	3.87−4	−6

T/K	A_1	A_2	A_3	A_4	Uncert.
146.4–304.1	1.726 31+1	−1.536 82	6.773 24−1		III
146.4–304.1	1.718 75+1	−1.458 79	6.576 59−1		III

Deviation plot for 2,2–Dichloro—1,1,1–trifluoroethane (25–038) is given in Fig. 62.

6.3.5.3. 1-Bromo-4-iodobenzene (25-051)

Name:	1-Bromo-4-iodobenzene
Formula:	C_6H_4BrI
CAS-RN:	589-87-7
Group No:	25-051

Experimental heat capacities (25.51.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001VAN/OON1		365.2–378.9	6	0.20	99.99	melpt	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (25.51.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	0.127	5.99−3	0.03	3.18−7	1

T/K	A_1	A_2	A_3	A_4	Uncert.
365.2–378.9	2.294 91−1	1.022 86+1	−1.050 55		I

6.4. Main group 3: compounds of carbon, hydrogen, and nitrogen

6.4.1. Sub group 31: amines

6.4.1.1. 1,2-Ethanediamine (31-004)

Name:	1,2-Ethanediamine
Formula:	$C_2H_8N_2$
CAS-RN:	107-15-3
Group No:	31-004

Experimental heat capacities (31.4.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1950HOU/MAS2		313.1–333.1	3	S	0.40	99.8	estim	*p*	BSAO	1950SAG/HOU
1975MES/FIN		293.2–334.3	10		0.20	99.9	melpt	sat	BSAO	1947HUF
1976NIC/SKO		298.1	1		0.20	n/a	n/a	*p*	DDCT	1971KON/SUU
1988BOB/KAM		313.1–413.1	6		6.00	97.	chrom	sat	BDCT	1986MER/BEN

6.4.1.2. 1-Propanamine (31-007)

Name:	1-Propanamine
Formula:	C_3H_9N
CAS-RN:	107-10-8
Group No:	31-007

Experimental heat capacities (31.7.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1967SMI/GOO2		298.1	1	n/a	99.972	melpt	*p*	n/a	n/a
1971KON/WAD		298.1	1	n/a	99.8	estim	*p*	BSIO	1970LKB/COM
1971VAS/PET		187.8–302.4	52	n/a	n/a	n/a	*p*	BSAO	1977KU/COM
1972FIN/MES		190.0–334.6	19	0.20	99.972	melpt	sat	BSAO	1947HUF
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

6.4.1.3. 1-Butanamine (31-010)

Name:	1-Butanamine
Formula:	$C_4H_{11}N$
CAS-RN:	109-73-9
Group No:	31-010

Experimental heat capacities (31.10.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1971KON/WAD		298.1	1	n/a	99.8	chrom	*p*	BSIO	1970LKB/COM
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

6.4.1.4. 1-Pentanamine (31-018)

Name:	1-Pentanamine
Formula:	$C_5H_{13}N$
CAS-RN:	110-58-7
Group No:	31-018

Experimental heat capacities (31.18.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1901KAH	N	329.1	1	n/a	n/a	n/a	avg	DSIO	1901KAH
1971KON/WAD		298.1	1	n/a	99.8	chrom	*p*	BSIO	1970LKB/COM
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

Reference	Notes
1901KAH	average value in the temperature range 294–364 K

6.4.1.5. Benzenamine (31-020)

Name:	Benzenamine
Formula:	C_6H_7N
CAS-RN:	62-53-3
Group No:	31-020

Experimental heat capacities (31.20.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1928LAN	N	274.2–332.0	14		n/a	n/a	n/a	*p*	FSIO	1928LAN
1931BLA/LEI		303.1–412.8	22		3.00	n/a	n/a	sat	BSIO	1931BLA/LEI
1933FER/MIL		291.6–322.8	12		1.00	n/a	n/a	sat	BDHO	1933FER/MIL
1933PAR/HUF		275.7–298.2	3		1.00	n/a	n/a	*p*	BSIO	1925PAR
1934RAD/JUL		288.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1937ELL		298.1–351.1	3	S	n/a	n/a	n/a	*p*	BSIO	1937ELL
1950HOU/MAS2		323.1–453.1	10	S	0.40	n/a	n/a	*p*	BSAO	1950SAG/HOU
1957CRU/JOS		293.1	1		2.00	n/a	n/a	*p*	BSIO	1957CRU/JOS
1962HAT/HIL		270.2–313.1	17		n/a	99.98	melpt	*p*	BSAO	1958HIL/KRA
1971DES/BHA		298.1–318.1	3	S	1.00	n/a	n/a	*p*	BSIO	1958MUR/VAN
1975NIC/WAD		298.1	1		n/a	99.5	chrom	*p*	BSIO	1970LKB/COM
1987LES/LIC		270.0–310.0	eqn		2.00	99.	estim	*p*	BDHT	1969PER/COM
1990RAO/RAJ		318.1–333.1	4		4.00	n/a	n/a	*p*	BDHT	1989PRA/RAJ
2002STE/CHI2		300.0–700.0	21	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1928LAN	corrected for water content (about 0.1 mass %)

Correlated heat capacities (31.20.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1962HAT/HIL	270.2–313.1	17	0.30	#	0.486	3.33−2	0.15	8.65−5	−1
1975NIC/WAD	298.1	1	0.50	#	0.461	5.30−2	0.23	−5.30−2	−1
2002STE/CHI2	300.0–680.0	20	1.00		0.778	2.78−1	0.78	1.58−2	6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1928LAN	(2.77−1, 1.18, 2.09−1, 10)	1931BLA/LEI	(1.82, 6.32, 1.37, 22)
1933FER/MIL	(2.31−1, 0.99, 2.29−1, 12)	1933PAR/HUF	(1.32−1, 0.58, −1.13−1, −3)
1934RAD/JUL	(7.38−1, 3.34, −7.38−1, −1)	1937ELL	(4.37−1, 1.78, 3.68−1, 3)
1950HOU/MAS2	(3.36−1, 1.31, −3.90−2, 2)	1957CRU/JOS	(1.66−1, 0.72, 1.66−1, 1)
1971DES/BHA	(5.11−1, 2.14, 4.82−1, 3)	1990RAO/RAJ	(1.32, 5.10, 9.13−1, 2)

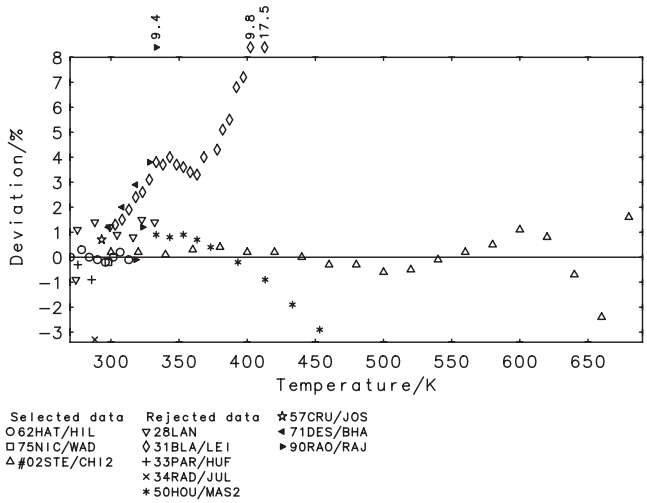

FIG. 63. Deviation plot for benzenamine (31-020).

Parameters of cubic spline polynomials (31.20.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	112	38	0.714	2.21−1	0.63	6.97−3	4
sat	112	38	0.552	1.42−1	0.43	4.60−3	3

T/K	A_1	A_2	A_3	A_4	Uncert.
270.2–420.0	1.508 19+1	4.863 33	−1.215 48	1.603 21−1	II
420.0–570.0	6.151 82+1	−2.830 55+1	6.681 85	−4.664 52−1	III
570.0–680.0	−1.264 02+3	6.693 48+2	−1.157 13+2	6.691 17	IV
270.2–420.0	1.685 17+1	3.243 65	−7.292 02−1	1.126 10−1	II
420.0–570.0	5.679 03+1	−2.528 39+1	6.063 07	−4.264 59−1	II
570.0–680.0	−7.636 68+2	4.065 36+2	−6.969 48+1	4.003 83	III

Parameters of quasipolynomial equation (31.20.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	112	38	1.017	2.79−1	0.84	1.59−2	−1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
270.2–680.0	705.00	−2.683 52	1.656 57−1	1.683 71+1	1.047 45+1	1.734 37−1	9.532 96−4	IV

Deviation plot for Benzenamine (31–020) is given in Fig. 63.

6.4.1.6. Cyclohexanamine (31-022)

Name:	Cyclohexanamine
Formula:	$C_6H_{13}N$
CAS-RN:	108-91-8
Group No:	31-022

Experimental heat capacities (31.22.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1975BER/OLO		298.1	1	n/a	99.7	anal	*p*	DDCT	1974SUU/WAD
1979STE	N	298.1	1	n/a	n/a	n/a	*p*	n/a	n/a

Reference	Notes
1979STE	the origin of data unclear; 0.05 mol % water was detected

6.4.1.7. *N*,*N*-Diethylethanamine (31-023)

Name:	*N*,*N*-Diethylethanamine
Formula:	$C_6H_{15}N$
CAS-RN:	121-44-8
Group No:	31-023

Experimental heat capacities (31.23.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		319.7–330.0	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1965KAU/BIT		293.1–343.1	6		1.00	n/a	n/a	*p*	FSIO	1965KAU/BIT
1975BER/OLO		298.1	1		n/a	99.7	anal	*p*	DDCT	1974SUU/WAD
1980ROU/ROB		278.1–288.1	2		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1985HEP/KOO		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1993GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994GRO/ROU		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED
2002GOR/WAS		298.1	1		0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

Correlated heat capacities (31.23.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1965KAU/BIT	293.1–343.1	6	1.00		1.738	4.74−1	1.74	3.00−1	2
1975BER/OLO	298.1	1	1.00	#	0.871	2.28−1	0.87	−2.28−1	−1
1985HEP/KOO	298.1	1	0.50	#	1.650	2.16−1	0.82	−2.16−1	−1
1991GRO/ROU	298.1	1	0.50	#	2.578	3.37−1	1.29	−3.37−1	−1
1993GRO/ROU	298.1	1	0.50	#	3.206	4.17−1	1.60	−4.17−1	−1
1994GRO/ROU	298.1	1	0.50	#	2.532	3.31−1	1.27	−3.31−1	−1
2002GOR/WAS	298.1	1	0.20		2.941	1.56−1	0.59	1.56−1	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1881VON	(1.62, 5.99, −1.60, −3)

Parameters of regression polynomial (31.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	17	12	2.315	4.32−1	1.60	3.58−2	−2	
T/K		A_1		A_2		A_3	A_4	Uncert.
293.1–343.1		8.327 16−1		8.591 32				V

Deviation plot for *N*,*N*-Diethylethanamine (31-023) is given in Fig. 64.

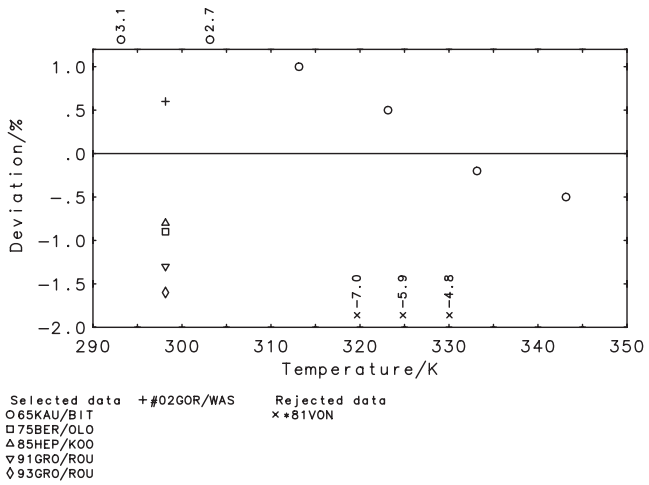

FIG. 64. Deviation plot for *N*,*N*-diethylethanamine (31-023).

6.4.1.8. 1-Hexanamine (31-024)

Name:	1-Hexanamine
Formula:	$C_6H_{15}N$
CAS-RN:	111-26-2
Group No:	31-024

Experimental heat capacities (31.24.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1971KON/WAD		298.1	1	n/a	99.8	chrom	*p*	BSIO	1970LKB/COM
1977BEL/BUB		298.1	1	n/a	n/a	n/a	*p*	BDCT	1968WAD
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO
2005DOM/MAR		267.3–295.6	27	n/a	98.0	chrom	*p*	BDCT	1989BRE/LIC

Correlated heat capacities (31.24.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1971KON/WAD	298.1	1	0.50	#	0.802	1.22−1	0.40	1.22−1	1
1977BEL/BUB	298.1	1	0.50	#	0.918	1.38−1	0.46	−1.38−1	−1
2002GOR/WAS	298.1	1	0.20		0.022	1.32−3	0.00	1.32−3	0
2005DOM/MAR	267.3–295.6	27	0.50	#	0.077	1.16−2	0.04	3.89−4	0

Parameters of regression polynomial (31.24.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	30	30	0.247	3.72−2	0.12	−1.49−4	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
267.3–298.1		3.368 53+1		−3.560 98		8.008 17−1		II

Deviation plot for 1-Hexanamine (31-024) is given in Fig. 65.

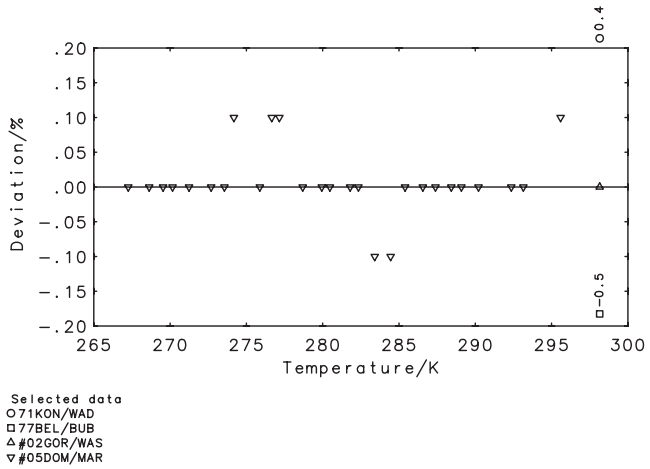

FIG. 65. Deviation plot for 1-hexanamine (31-024).

6.4.1.9. *N*-Propyl-1-propanamine (31-025)

Name:	*N*-Propyl-1-propanamine
Formula:	$C_6H_{15}N$
CAS-RN:	142-84-7
Group No:	31-025

Experimental heat capacities (31.25.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1901KAH	N	334.1	1	n/a	n/a	n/a	avg	DSIO	1901KAH
1975BER/OLO		298.1	1	n/a	99.7	anal	*p*	DDCT	1974SUU/WAD
1991PES/NIK	N	298.1	1	n/a	n/a	n/a	*p*	BSAO	1983KUK/KOR

Reference	Notes
1901KAH	average value in the temperture range 294–374 K
1991PES/NIK	water content below 0.05%

6.4.1.10. 1-Octanamine (31-053)

Name:	1-Octanamine
Formula:	$C_8H_{19}N$
CAS-RN:	111-86-4
Group No:	31-053

Experimental heat capacities (31.53.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1982PFE/KUC		298.1	1	n/a	n/a	n/a	*p*	BDCT	1968WAD
1993STE/CHI2	N	300.0–620.0	17	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO
2005DOM/MAR		295.1–313.2	36	n/a	98.0	chrom	*p*	BDCT	1989BRE/LIC

Reference	Notes
1993STE/CHI2	same data in 1996STE/CHI2

6.4.1.11. 1-Decanamine (31-061)

Name:	1-Decanamine
Formula:	$C_{10}H_{23}N$
CAS-RN:	2016-57-1
Group No:	31-061

Experimental heat capacities (31.61.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1977BEL/BUB		298.1	1	n/a	n/a	n/a	p	BDCT	1968WAD
2005DOM/MAR		298.1–333.3	36	n/a	95.0	chrom	p	BDCT	1989BRE/LIC

Correlated heat capacities (31.61.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1977BEL/BUB	298.1	1	2.00	#	1.160	1.07	2.32	1.07	1
2005DOM/MAR	298.1–333.3	36	0.30	#	0.188	2.55−2	0.06	−6.05−4	5

Parameters of regression polynomial (31.61.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	37	37	0.277	1.85−1	0.40	2.82−2	6	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.1–333.3		6.137 58+1		−1.312 37+1		2.546 84		II

Deviation plot for 1-Decanamine (31-061) is given in Fig. 66.

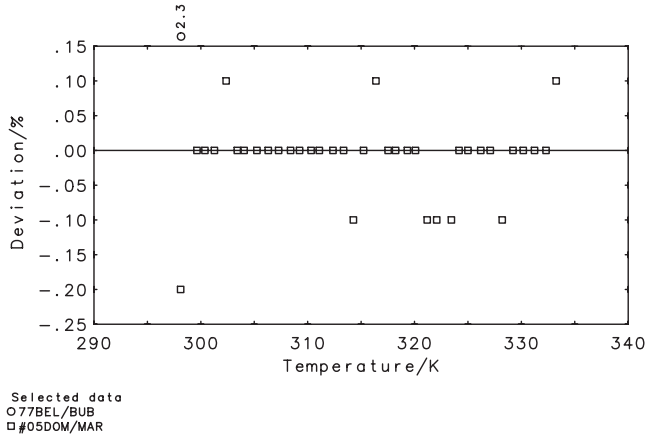

FIG. 66. Deviation plot for 1-decanamine (31-061).

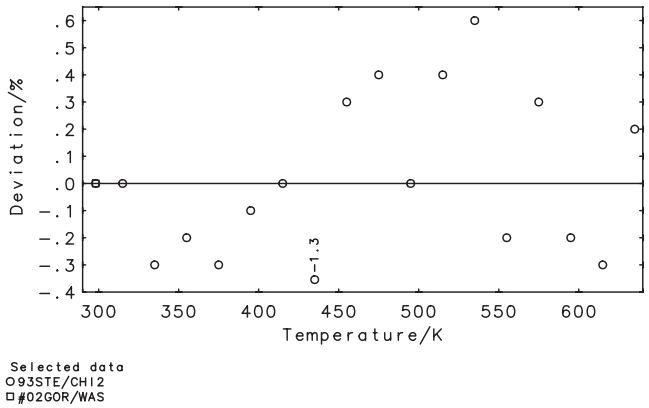

FIG. 67. Deviation plot for *N*,*N*-dioctyl-1-octanamine (31-065).

6.4.1.12. *N*,*N*-Dioctyl-1-octanamine (31-065)

Name:	*N*,*N*-Dioctyl-1-octanamine
Formula:	$C_{24}H_{51}N$
CAS-RN:	1116-76-3
Group No:	31-065

Experimental heat capacities (31.65.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993STE/CHI2	N	298.1–635.0	18	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2002GOR/WAS		298.1	1	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

Reference	Notes
1993STE/CHI2	same data in 1996STE/CHI2

Correlated heat capacities (31.65.2)

Reference	*T*/K	nPts	$\sigma_r C$/%	d_w	*d*/R	d_r/%	d_b/R	+/−
1993STE/CHI2	298.1–635.0	18	1.00	0.406	4.71−1	0.41	−4.15−2	−5
2002GOR/WAS	298.1	1	0.20	0.189	3.41−2	0.04	3.41−2	1

Parameters of regression polynomial (31.65.3)

Type	nTot	nPts	s_w	*s*/R	s_r/%	s_b/R	+/−	
C	19	19	0.420	4.84−1	0.42	−3.76−2	−4	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.1–635.0		4.452 01+1		1.536 88+1				III

Deviation plot for *N*,*N*-Dioctyl-1-octanamine (31-065) is given in Fig. 67.

6.4.1.13. 1,3-Propanediamine (31-066)

Name:	1,3-Propanediamine
Formula:	$C_3H_{10}N_2$
CAS-RN:	109-76-2
Group No:	31-066

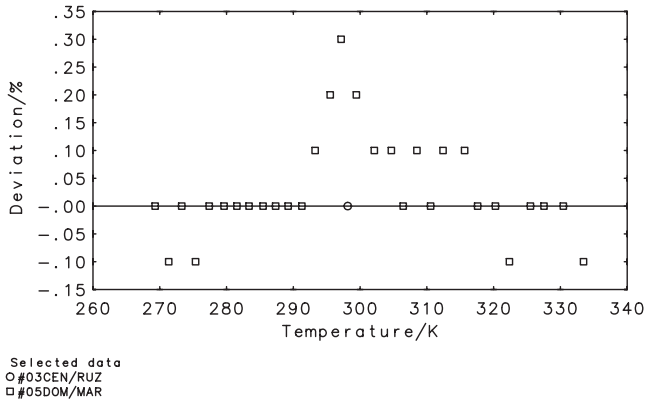

FIG. 68. Deviation plot for 1,3-propanediamine (31-066).

Experimental heat capacities (31.66.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003CEN/RUZ		298.1	1	0.20	n/a	n/a	p	BDCT	1991BAN/GAR
2005DOM/MAR		269.3–333.5	30	n/a	99.0	chrom	p	BDCT	1989BRE/LIC

Correlated heat capacities (31.66.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2003CEN/RUZ	298.1	1	0.20		0.198	9.72−3	0.04	−9.72−3	−1
2005DOM/MAR	269.3–333.5	30	1.00	#	0.092	2.25−2	0.09	8.15−3	7

Parameters of regression polynomial (31.66.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	31	31	0.100	2.30−2	0.09	7.57−3	6

T/K	A_1	A_2	A_3	A_4	Uncert.
269.3–333.5	2.009 14+1	1.485 77			I

Deviation plot for 1,3–Propanediamiine (31-066) is given in Fig. 68.

6.4.1.14. *N*,*N*-Dipropyl-1-propanamine (31-067)

Name:	*N*,*N*-Dipropyl-1-propanamine
Formula:	$C_9H_{21}N$
CAS-RN:	102-69-2
Group No:	31-067

Experimental heat capacities (31.67.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002GOR/WAS		298.15	2.101	0.20	99.5	chrom	p	BDCT	2000ERN/CHO

6.4.1.15. *N*,*N*-Dibutyl-1-butanamine (31-068)

Name:	*N*,*N*-Dibutyl-1-butanamine
Formula:	$C_{12}H_{27}N$
CAS-RN:	102-82-9
Group No:	31-068

Experimental heat capacities (31.68.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002GOR/WAS		298.15	2.114	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

6.4.1.16. *N*,*N*-Dihexyl-1-hexanamine (31-069)

Name:	*N*,*N*-Dihexyl-1-hexanamine
Formula:	$C_{18}H_{39}N$
CAS-RN:	102-86-3
Group No:	31-069

Experimental heat capacities (31.69.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002GOR/WAS		298.15	2.10	0.20	99.5	chrom	*p*	BDCT	2000ERN/CHO

6.4.2. Subgroup 32: nitriles

6.4.2.1. Benzonitrile (32-021)

Name:	Benzonitrile
Formula:	C_7H_5N
CAS-RN:	100-47-0
Group No:	32-021

Experimental heat capacities (32.21.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1900LOU	N	376.6	1	n/a	n/a	n/a	avg	DSIO	1898LOU
1983BYK/LEB2	N	265.3–328.9	14	0.30	99.88	melpt	*p*	BSAO	1976LEB/LIT
1985LAI/ROD		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1985TAN/NAK		283.1–318.1	3	0.30	99.9	chrom	*p*	FSIT	1971PIC/LED
1987MIR/SHA		273.0–453.0	10	1.90	n/a	n/a	*p*	BDHT	1984GUS/MIR
1997TAN/NAK	N	298.1–303.1	2	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1998WIL/EGG		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED

Reference	Notes
1900LOU	average value in the temperature range 294–459 K
1983BYK/LEB2	smoothed values in 1984LEB/BYK2
1997TAN/NAK	sample contained a small amount of water <0.1%

6.4.2.2. 4-(*trans*-4-Propylcyclohexyl)benzonitrile (32-031)

Name:	4-(*trans*-4-Propylcyclohexyl)benzonitrile
Formula:	$C_{16}H_{21}N$
CAS-RN:	61203-99-4
Group No:	32-031

Experimental heat capacities (32.31.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1998ASA/SOR		319.6–385.2	63	n/a	99.8	melpt	p	BSAO	1992SOR/KAJ

Parameters of cubic spline polynomials (32.31.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	63	63	0.420	2.20−1	0.42	1.70−3	−14

T/K	A_1	A_2	A_3	A_4	Uncert.
319.6–335.0	2.235 19+4	−1.997 29+4	5.961 05+3	−5.928 76+2	II
335.0–385.2	−5.925 04+1	9.682 90+1	−2.990 31+1	3.238 86	II

6.4.3. Subgroup 33: heterocyclic nitrogen compounds

6.4.3.1. Pyrazine (33-057)

Name:	Pyrazine
Formula:	$C_4H_4N_2$
CAS-RN:	290-37-9
Group No:	33-057

Experimental heat capacities (33.57.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI3		360.0–580.0	12	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2003CHI/KNI		329.5–386.3	7		0.10	99.985	melpt	sat	BSAO	1988STE/ARC

Correlated heat capacities (33.57.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002STE/CHI3	360.0–580.0	12	1.00	0.265	5.69−2	0.27	−2.86−3	0
2003CHI/KNI	329.5–386.3	7	0.10	0.109	1.84−3	0.01	5.48−5	1

Parameters of cubic spline polynomials (33.57.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.257	5.27−2	0.25	−1.78−3	1
sat	19	19	0.221	4.18−2	0.20	−1.67−3	1

T/K	A_1	A_2	A_3	A_4	Uncert.
329.5–480.0	1.657 29+1	−3.749 95	1.483 96	−1.116 75−1	II
480.0–580.0	−3.631 89+2	2.336 01+2	−4.796 42+1	3.322 22	III
329.5–480.0	1.716 12+1	−4.353 56	1.689 09	−1.347 70−1	II
480.0–580.0	−2.534 09+2	1.647 53+2	−3.354 14+1	2.311 79	III

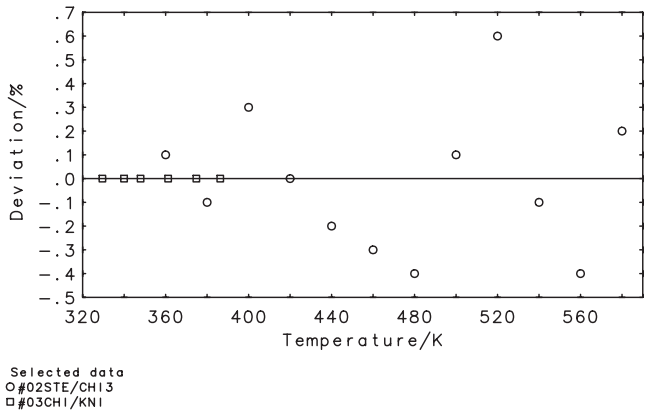

FIG. 69. Deviation plot for pyrazine (33-057).

Parameters of quasi-polynomial equation (33.57.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	1.117	3.42−2	0.18	−3.50−3	−3

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
329.5–580.0	627.00	−2.585 25−1	4.886 59−1	2.150 69	3.719 56+1	−2.880 98+1	9.278 07	IV

Deviation plot for Pyrazine (33–057) is given in Fig. 69.

6.4.3.2. 2-Methylquinoline (33-058)

Name:	2-Methylquinoline
Formula:	$C_{10}H_9N$
CAS-RN:	91-63-4
Group No:	33-058

Experimental heat capacities (33.58.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CHI/STE1		272.7–439.5	10	0.10	99.96	melpt	sat	BSAO	1988STE/ARC
2005CHI/STE1		460.0–700.0	13	1.00	99.96	melpt	sat	BSAO	1989KNI/ARC

Correlated heat capacities (33.58.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2005CHI/STE1	272.7–439.5	10	0.10	0.768	2.06−2	0.08	−8.02−4	1
2005CHI/STE1	460.0–700.0	13	1.00	0.407	1.68−1	0.41	7.36−2	7

Parameters of regression polynomial (33.58.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	23	23	0.619	1.33−1	0.32	4.13−2	8

T/K	A_1	A_2	A_3	A_4	Uncert.
272.7–700.0	1.216 44+1	4.955 15			III

Deviation plot for 2–Methylquinoline (33–058) is given in Fig. 70.

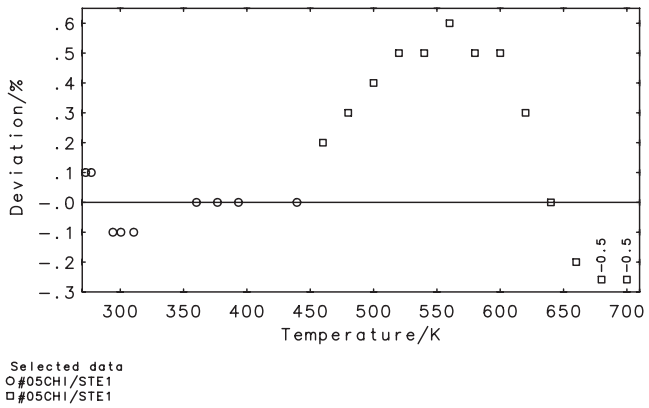

FIG. 70. Deviation plot for 2-methylquinoline (33-058).

6.4.3.3. 8-Methylquinoline (33-059)

Name:	8-Methylquinoline
Formula:	$C_{10}H_9N$
CAS-RN:	611-32-5
Group No:	33-059

Experimental heat capacities (33.59.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CHI/STE1		282.8–437.1	12	0.10	99.88	melpt	sat	BSAO	1988STE/ARC
2005CHI/STE1		440.0–700.0	14	1.00	99.88	melpt	sat	BSAO	1989KNI/ARC

Correlated heat capacities (33.59.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2005CHI/STE1	282.8–437.1	12	0.10	0.971	2.78−2	0.10	1.01−3	0
2005CHI/STE1	440.0–700.0	14	1.00	0.470	2.07−1	0.47	−7.88−2	2

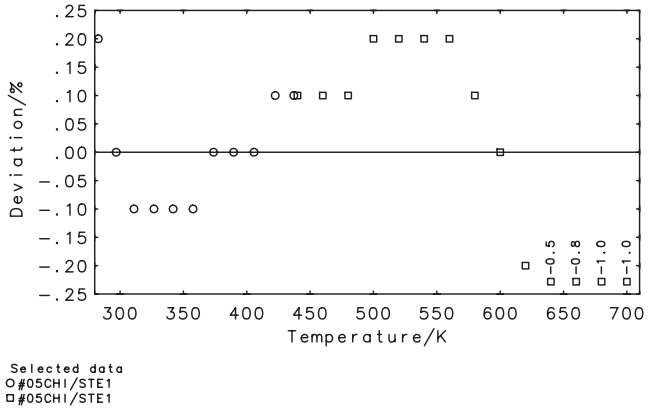

FIG. 71. Deviation plot for 8-methylquinoline (33-059).

Parameters of regression polynomial (33.59.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−	
Sat	26	26	0.791	1.63−1	0.37	−4.19−2	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
282.8–700.0		1.129 70+1		5.446 17		−7.502 32−2		IV

Deviation plot for 8–Methylquinoline (33–059) is given in Fig. 71.

6.4.3.4. 1-Methyl-3,5-diphenyl-1*H*-pyrazole (33-060)

Name: 1-Methyl-3,5-diphenyl-1*H*-pyrazole

Formula: $C_{16}H_{14}N_2$
CAS-RN: 19311-79-6
Group No: 33-060

Experimental heat capacities (33.60.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001DI/SUN1		335.2–369.4	14	0.25	99.54	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (33.60.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−	
p	14	14	1.122	1.31−1	0.28	5.71−4	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
335.2–369.4		8.767 77		1.097 27+1				III

6.4.4. Subgroup 34: miscellaneous nitrogen compounds

6.4.4.1. 3-(Phenylamino)propanenitrile (34-015)

Name: 3-(Phenylamino)propanenitrile

Formula: $C_9H_{10}N_2$
CAS-RN: 1075-76-9
Group No: 34-015

Experimental heat capacities (34.15.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005TIA/TAN		324.8–353.1	25	0.50	99.0	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (34.15.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−	
p	25	24	0.506	8.05−2	0.25	5.16−3	−3	
T/K		A_1		A_2		A_3	A_4	Uncert.
325.9–353.1		−1.976 82+4		1.797 45+4		−5.440 89+3	5.491 06+2	III

6.5. Main group 4: compounds of carbon, hydrogen, and oxygen

6.5.1. Subgroup 41: ethers

6.5.1.1. 1,2-Dimethoxyethane (41-007)

Name:	1,2-Dimethoxyethane
Formula:	$C_4H_{10}O_2$
CAS-RN:	110-71-4
Group No:	41-007

Experimental heat capacities (41.7.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1973KUS/SUU		298.1	1	0.10	n/a	n/a	p	DDCT	1971KON/SUU
1990TRE	N	298.1	1	n/a	n/a	n/a	p	FSIT	1971PIC/LED
1991TRE/COS		298.1	1	n/a	99.	anal	p	FSIT	1971PIC/LED
1996STE/CHI3	N	315.0–535.0	12	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
1999BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	p	FSIO	1999BUR/ZOC
2001BAL/MAT		298.1	1	n/a	n/a	n/a	p	FSIO	1985OGA

Reference	Notes
1990TRE	measured by P. Y. D'Arcy and C. Y. Halpin (personal communication)
1996STE/CHI3	value at 535 K was not included in fit; heat capacity shows large drop on passing into the fluid phase

6.5.1.2. 2-Methoxy-2-methylpropane (41-010)

Name:	2-Methoxy-2-methylpropane
Formula:	$C_5H_{12}O$
CAS-RN:	1634-04-4
Group No:	41-010

Experimental heat capacities (41.10.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936EVA/EDL		298.1	1	n/a	n/a	n/a	p	n/a	n/a
1975AND/MAR		168.3–308.4	38	n/a	99.95	melpt	p	BSAO	1963AND/COU1
2004PAR/ZOU		277.1–325.1	25	0.30	99.5	anal	sat	BDCT	1983ROU/ROU

Correlated heat capacities (41.10.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936EVA/EDL	298.1	1	1.00	#	0.125	2.82−2	0.12	−2.82−2	−1
1975AND/MAR	168.3–308.4	38	1.00	#	0.223	4.93−2	0.22	−1.88−2	4
2004PAR/ZOU	277.1–325.1	25	0.30		0.460	3.13−2	0.14	2.78−3	3

Parameters of regression polynomial (41.10.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	64	64	0.343	4.39−2	0.20	−1.05−2	6

T/K	A_1	A_2	A_3	A_4	Uncert.
168.3–325.1	1.781 57+1	−9.982 40−1	8.787 69−1		II

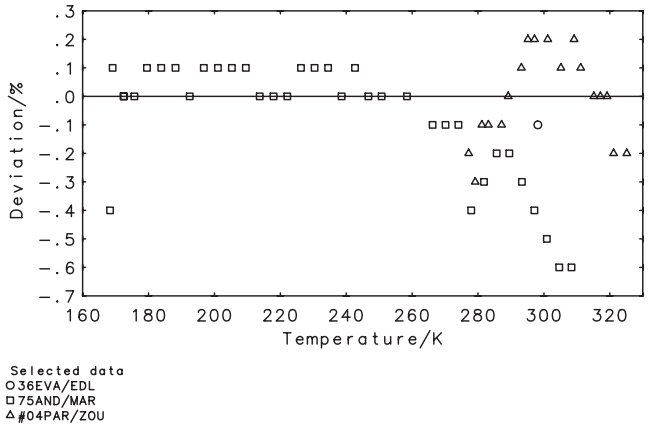

FIG. 72. Deviation plot for 2-methoxy-2-methylpropane (41-010).

Parameters of quasi-polynomial equation (41.10.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	64	64	0.376	4.11−2	0.18	−3.01−3	11

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
168.3–325.1	497.10	5.570 04	1.169 78−1	1.688 30+1	6.528 79	9.328 39	1.524 90+1	II

Deviation plot for 2–Methoxy—2–methylpropane (41–010) is given in Fig. 72.

6.5.1.3. 2-Ethoxy-2-methylpropane (41-015)

Name:	2-Ethoxy-2-methylpropane
Formula:	$C_6H_{14}O$
CAS-RN:	637-92-3
Group No:	41-015

Experimental heat capacities (41.15.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936EVA/EDL		298.1	1		n/a	n/a	n/a	*p*	n/a	n/a
2004DRU/VAR		179.3–340.0	19	S	0.20	99.91	melpt	*p*	BSAO	1997VAR/DRU1
2004PAR/ZOU		277.1–341.1	32		0.30	97.0	anal	sat	BDCT	1983ROU/ROU

Correlated heat capacities (41.15.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004DRU/VAR	179.3–340.0	19	0.20	0.953	5.32−2	0.19	−2.50−2	−9
2004PAR/ZOU	277.1–341.1	32	0.30	0.652	5.31−2	0.20	3.38−2	23

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1936EVA/EDL	(2.69−1, 1.03, −2.69−1, −1)

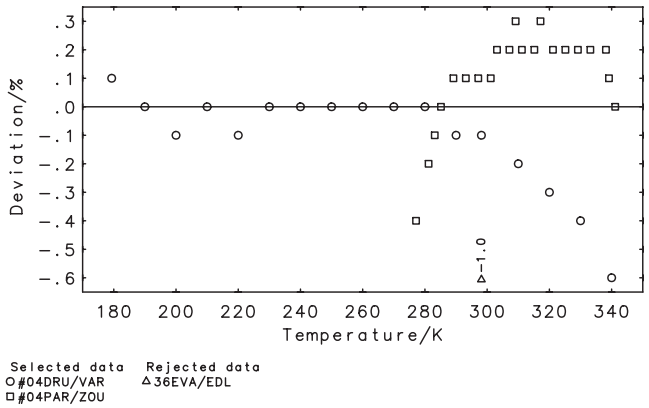

FIG. 73. Deviation plot for 2-ethoxy-2-methylpropane (41-015).

Parameters of regression polynomial (41.15.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−	
C	52	51	0.802	5.48-2	0.20	1.19−2	14	
T/K		A_1		A_2		A_3	A_4	Uncert.
179.3–341.1		1.785 78+1		1.082 12		6.083 35−1		IV

Deviation plot for 2–Ethoxy—2–methylpropane (41–015) is given in Fig. 73.

6.5.1.4. 2-Methoxy-2-methylbutane (41-016)

Name:	2-Methoxy-2-methylbutane
Formula:	$C_6H_{14}O$
CAS-RN:	994-05-8
Group No:	41-016

Experimental heat capacities (41.16.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936EVA/EDL		298.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1991ROZ/SAF		298.1	1		n/a	99.6	chrom	*p*	BDHT	1969PER/COM
2002STE/CHI1		300.0–500.0	11	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2004PAR/ZOU		279.2–355.1	39		0.30	97.0	anal	sat	BDCT	1983ROU/ROU

Correlated heat capacities (41.16.2)

Reference	T/K	nPts	$\sigma_r C/\%$	d_w	d/R	$d_r/\%$	d_b/R	+/−
2002STE/CHI1	300.0–500.0	11	1.00	0.725	2.41−1	0.73	−4.27−2	−3
2004PAR/ZOU	279.2–355.1	39	0.30	0.179	1.42−2	0.05	1.19−3	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1936EVA/EDL	(9.11−1, 3.41, 9.11−1, 1)	1991ROZ/SAF	(5.93, 29.80, −5.93, −1)

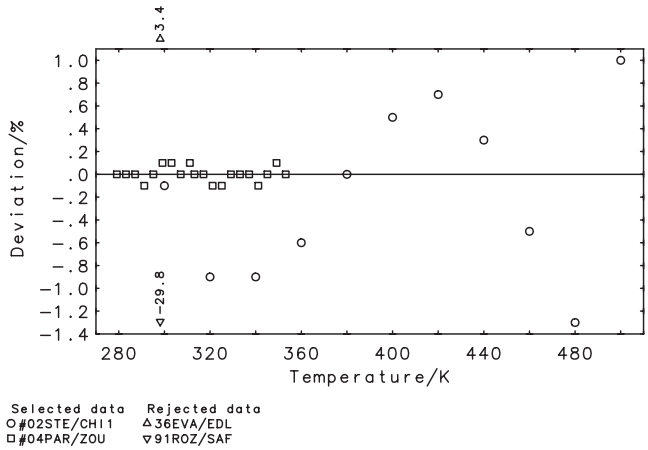

FIG. 74. Deviation plot for 2-methoxy-2-methylbutane (41-016).

Parameters of regression polynomial (41.16.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	52	50	0.391	1.18−1	0.36	−8.46−3	−4
sat	52	50	0.376	9.94−2	0.32	−3.74−3	−6

T/K	A_1	A_2	A_3	A_4	Uncert.
279.2–500.0	−1.710 35+1	3.106 42+1	−7.971 24	7.987 67−1	III
279.2–500.0	−6.978 62	2.171 91+1	−5.102 09	5.054 75−1	III

Parameters of quasi-polynomial equation (41.16.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	52	50	0.572	9.20−2	0.31	−1.13−2	8

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
279.2-500.0	537.00	−2.905 00	1.366 22−1	1.347 72+1	1.816 34+1	−1.294 31	3.113 10−2	III

Deviation plot for 2–Methyoxy—2–methylbutane (41–016) is given in Fig. 74.

6.5.1.5. 2,2′-Oxybis(propane) (41-018)

Name:	2,2′-Oxybis(propane)
Formula:	$C_6H_{14}O$
CAS-RN:	108-20-3
Group No:	41-018

Experimental heat capacities (41.18.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1933PAR/HUF		194.5–293.1	8		1.00	n/a	n/a	p	BSIO	1925PAR
1961ROU	N	296.1–318.1	2		n/a	n/a	n/a	p	BSAO	1961ROU
1974AND/COU		187.8–340.0	19	S	n/a	99.86	melpt	p	BSAO	1963AND/COU1
1990TRE	N	298.1	1		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1991GRO/ROU		298.1	1		n/a	99.	anal	p	FSIT	1971PIC/LED
1993GRO/ROU		298.1	1		n/a	99.0	anal	p	FSIT	1971PIC/LED
1994GRO/ROU		298.1	1		n/a	99.5	anal	p	FSIT	1971PIC/LED
2004PAR/ZOU		277.2–337.1	31		0.30	99.0	anal	sat	BDCT	1983ROU/ROU

Reference	Notes
1961ROU	constant value in the temperature range 296–318 K obtained by the author
1990TRE	measured by P. Y. D'Arcy and C. Y. Halpin (personal communication)

6.5.1.6. 2-Ethoxy-2-methylbutane (41-024)

Name:	2-Ethoxy-2-methylbutane
Formula:	$C_7H_{16}O$
CAS-RN:	919-94-8
Group No:	41-024

Experimental heat capacities (41.24.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936EVA/EDL		298.1	1		n/a	n/a	n/a	p	n/a	n/a
2004DRU/VAR		157.7–340.0	21	S	0.20	99.87	melpt	p	BSAO	1997VAR/DRU1

Correlated heat capacities (41.24.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936EVA/EDL	298.1	1	1.00	#	1.561	4.56−1	1.56	−4.56−1	−1
2004DRU/VAR	157.7–340.0	21	0.20		0.439	2.61−2	0.09	9.27−4	4

Parameters of regression polynomial (41.24.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	22	22	0.585	1.08−1	0.37	−1.99−2	3	
T/K		A_1		A_2		A_3	A_4	Uncert.
157.7–340.0		2.165 86+1		2.031 31−1		8.358 36−1		II

Deviation plot for 2–Ethoxy—2–methylbutane (41–024) is given in Fig. 75.

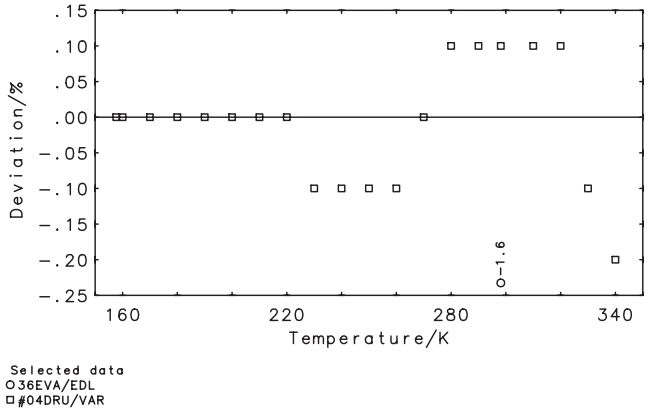

FIG. 75. Deviation plot for 2-ethoxy-2-methylbutane (41-024).

6.5.1.7. 2,5,8,11-Tetraoxadodecane (41-037)

Name:	2,5,8,11-Tetraoxadodecane
Formula:	$C_8H_{18}O_4$
CAS-RN:	112-49-2
Group No:	41-037

Experimental heat capacities (41.37.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1966BEA/CLE		230.0–350.0	14	n/a	99.44	melpt	*p*	BSAO	1933SOU/BRI
1985BEN/KUM		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1990TRE	N	298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991TRE/COS		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1997TOV/CAR1		283.1–308.1	4	n/a	n/a	n/a	*p*	BDHT	1969PER/COM
1997TOV/CAR3	N	288.1–308.1	3	n/a	99.0	anal	*p*	BDCT	1983ROU/ROU
1999BUR/ZOC		298.1–323.1	2	2.00	99.5	chrom	*p*	FSIO	1999BUR/ZOC
2001BEC/GME		310.1–415.1	22	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Reference	Notes
1990TRE	measured by P. Y. D'Arcy and C. J. Halpin (personal communication)
1997TOV/CAR3	same data for temperatures 288.15 and 298.15 K in 1997TOV/CAR1

Correlated heat capacities (41.37.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1966BEA/CLE	230.0–350.0	14	1.50	#	0.156	1.04−1	0.23	−1.81−2	−2
1985BEN/KUM	298.1	1	0.50	#	0.072	1.60−2	0.04	−1.60−2	−1
1991TRE/COS	298.1	1	0.50	#	0.189	4.18−2	0.09	4.18−2	1
1997TOV/CAR1	283.1–308.1	4	0.50	#	1.227	2.73−1	0.61	2.71−1	4
1997TOV/CAR3	288.1–308.1	3	0.50	#	1.147	2.55−1	0.57	2.55−1	3
2001BEC/GME	310.1–415.1	22	0.50		0.657	1.46−1	0.33	−3.91−2	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1990TRE	(1.03−1, 0.23, −1.03−1, −1)	1999BUR/ZOC	(4.44−1, 0.99, 4.11−1, 2)

Parameters of regression polynomial (41.37.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	48	45	0.665	1.77−1	0.40	−2.83−2	4

T/K	A_1	A_2	A_3	A_4	Uncert.
230.0–415.1	5.951 12+1	−1.052 35+1	1.502 52	1.046 49−1	IV

Parameters of quasipolynomial equation (41.37.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	48	35	0.676	1.62−1	0.36	3.05−2	11

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
290.0–410.0	651.00	1.262 88+3	1.085 23+2	−1.168 04+2	1.590 84+3	−7.446 43+2	1.684 52+3	V

Deviation plot for 2,5,8,11–Tetraoxadodecane (41–037) is given in Fig. 76.

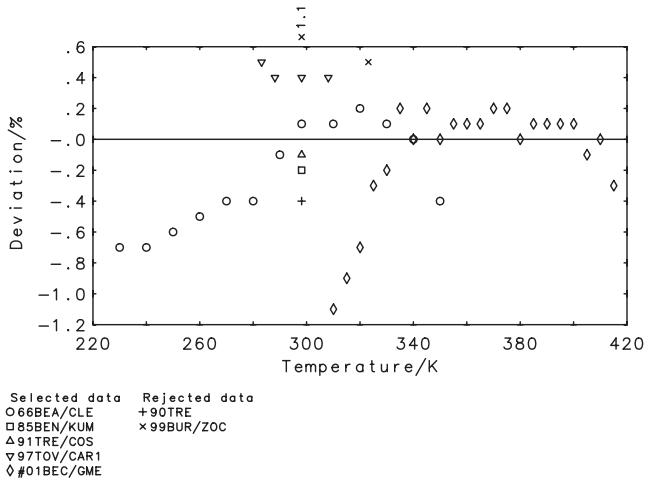

FIG. 76. Deviation plot for 2,5,8,11-tetraoxadodecane (41-037).

6.5.1.8. 2-Methyl-2-(1-methylethoxy)propane (41-052)

Name:	2-Methyl-2-(1-methylethoxy)propane
Formula:	$C_7H_{16}O$
CAS-RN:	17348-59-3
Group No:	41-052

Experimental heat capacities (41.52.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001VAR/DRU		186.6–354.6	125	0.30	99.11	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (41.52.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	125	125	0.518	4.67−2	0.16	1.48−4	10	
T/K		A_1		A_2		A_3	A_4	Uncert.
186.6–354.6		1.939 94+1		1.720 44		5.639 21−1		II

Parameters of quasipolynomial equation (41.52.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−					
p	125	125	0.497	4.40−2	0.15	1.28−4	5					
T/K		T_c/K	A_1		A_2		A_3	A_4	A_5	A_6	Uncert.	
186.6–354.6		520.00	−4.401 42		2.786 63−1		1.769 60+1	1.157 04+1	2.331 87	1.476 84−1	II	

6.5.1.9. 2-Methyl-2-propoxypropane (41-053)

Name:	2-Methyl-2-propoxypropane
Formula:	$C_7H_{16}O$
CAS-RN:	29072-93-3
Group No:	41-053

Experimental heat capacities (41.53.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001VAR/DRU		181.1–353.1	92	0.30	99.45	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (41.53.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	92	92	0.383	3.21−2	0.11	5.71−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
181.1–353.1	1.998 67+1	1.150 19	6.618 99−1		II

Parameters of quasipolynomial equation (41.53.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	92	92	0.328	2.80−2	0.10	5.08−5	14

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
181.1–353.1	533.00	2.333 00+1	1.088 36	1.963 94+1	2.629 58+1	2.483 52+1	2.200 38+1	II

6.5.1.10. 1,2-Dimethoxybenzene (41-054)

Name: 1,2-Dimethoxybenzene

Formula: $C_8H_{10}O_2$
CAS-RN: 91-16-7
Group No: 41-054

Experimental heat capacities (41.54.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001BEC/GME		310.0–415.1	22	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Parameters of regression polynomial (41.54.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	22	22	0.169	3.07−2	0.08	4.89−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
310.0–415.1	1.195 18+2	1.185 98+2	−3.080 47+1	2.741 96	II

6.5.1.11. 1-(1,1-Dimethylethoxy)-2-methylpropane (41-055)

Name: 1-(1,1-Dimethylethoxy)-2-methylpropane

Formula: $C_8H_{18}O$
CAS-RN: 33021-02-2
Group No: 41-055

Experimental heat capacities (41.55.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DRU/DOR		163.9–353.4	165	0.30	99.92	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (41.55.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	165	165	0.518	4.74−2	0.16	1.48−4	4

T/K	A_1	A_2	A_3	A_4	Uncert.
163.9–353.4	2.093 51+1	2.124 80	5.700 58−1		III

6.5.1.12. 1,1′-[Methylenebis(oxy)]bis(butane) (41-056)

Name: 1,1′-[Methylenebis(oxy)]bis(butane)

Formula: $C_9H_{20}O_2$
CAS-RN: 2568-90-3
Group No: 41-056

Experimental heat capacities (41.56.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000PAL/SZA		293.1–416.1	22	n/a	99.98	anal	p	BDHT	1973PER/COM

Parameters of regression polynomial (41.56.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	22	22	0.081	3.68−2	0.08	−1.14−4	4

T/K	A_1	A_2	A_3	A_4	Uncert.
293.1–416.1	1.398 52+1	8.780 08	I		

6.5.1.13. 2,3,6,7,10,11-Hexahexyloxytriphenylene (41-057)

Name: 2,3,6,7,10,11-Hexahexyloxytriphenylene

Formula: $C_{54}H_{84}O_6$
CAS-RN: 70351-86-9
Group No: 41-057

Experimental heat capacities (41.57.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1990SOR/ASA		372.3–397.1	18	n/a	99.3	melpt	p	BSAO	1992SOR/KAJ

Parameters of regression polynomial (41.57.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	18	18	0.234	2.59−1	0.12	5.06−4	2

T/K	A_1	A_2	A_3	A_4	Uncert.
372.3–397.1	2.756 86+2	−5.824 07+1	1.165 03+1		II

6.5.2. Sub group 42: alcohols and phenols

6.5.2.1. Methanol (42-002)

Name:	Methanol
Formula:	CH_4O
CAS-RN:	67-56-1
Group No:	42-002

Experimental heat capacities (42.2.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1907WAL		292.1	1		n/a	n/a	n/a	avg	DSIO	1907WAL
1925DRU/WEI		293.1	1		n/a	n/a	n/a	*p*	BSIO	1925DRU/WEI
1925PAR		188.4–290.1	8		0.50	n/a	n/a	*p*	BSIO	1925PAR
1929KEL1		181.1–292.0	14		1.00	n/a	n/a	*p*	BSIO	1929KEL1
1929MIT/HAR1		190.5–264.8	18		n/a	n/a	n/a	*p*	BSIO	1929MIT/HAR1
1931FIO/GIN	N	318.1–378.1	7	S	0.10	99.97	estim	sat	BSIO	1931FIO/GIN
1939PHI		300.8	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1949STA/GUP		180.0–270.0	10	S	0.50	n/a	n/a	*p*	BSAO	1949STA/GUP
1949TSC/RIC2		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1950HOU/MAS2		323.1–353.1	4	S	0.40	99.8	estim	*p*	BSAO	1950SAG/HOU
1960SWI/ZIE	N	311.6	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1962KAT		283.1–333.1	4		n/a	n/a	n/a	*p*	BSIO	1962KAT
1966DRA/LAN	N	298.1	1		n/a	n/a	n/a	*p*	BSIO	1966DRA/LAN
1968PAZ/REC	N	313.1	1		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1971CAR/WES		180.0–320.0	17	S	n/a	99.975	melpt	*p*	BSAO	1968WES/FUR
1971DES/BHA		298.1–318.1	3	S	1.00	n/a	n/a	*p*	BSIO	1958MUR/VAN
1971GOP/GAM		308.0–333.0	eqn		1.00	n/a	n/a	*p*	BSAO	1971GOP/GAM
1981ATA/ELS		293.1	1		2.50	n/a	n/a	*p*	BDHO	1981ATA/ELS
1982BEN/DAR		288.1–308.1	2		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1982VIL/CAS		298.1	1		0.30	99.8	chrom	*p*	FSIT	1971PIC/LED
1984ZEG/SOM2		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1985COS/PAT8		298.1–313.1	2		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1986KOR/KUK		278.0–298.0	2		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1986OGA/MUR		298.1	1		0.10	n/a	n/a	*p*	FSIO	1985OGA
1986TAN/TOY		298.1	1		0.30	99.96	anal	*p*	FSIT	1971PIC/LED
1987LAN/CRI	N	298.1–313.1	2		n/a	n/a	n/a	*p*	FSIO	1987LAN/CRI
1988AND/PAT		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1988BOY/CRI	N	393.1–503.1	5		n/a	n/a	n/a	*p*	FSIO	1987LAN/CRI
1988OKA/OGA	N	298.1–299.1	2		n/a	n/a	n/a	*p*	FSIO	1985OGA
1989DOU/KHA		298.1	1		n/a	99.8	estim	*p*	FSIT	1971PIC/LED
1992FIL/AFA		298.1	1		n/a	n/a	n/a	*p*	BDCT	1992FIL/AFA
1993CON/GIR1		298.0–343.0	eqn		5.00	n/a	n/a	sat	BDHT	1993CON/GIR1
1993NAZ/BAS		298.1–325.5	2		2.20	99.5	anal	*p*	BDHO	1986NAZ/BAS1
1997RIG/COM		308.1	1		1.00	n/a	n/a	*p*	BDHT	1995DIO/MAN
2002PAR/ZOU		278.1–348.1	15		n/a	99.5	chrom	sat	BDCT	1983ROU/ROU

Reference	Notes
1931FIO/GIN	data calculated using procedure by 1985WIL/CHA
1960SWI/ZIE	average value in the temperature range 294–329 K
1966DRA/LAN	grade: pure, water content is 0.08%
1968PAZ/REC	same datum in 1970PAZ/PAZ
1987LAN/CRI	C_p at 298.15 K measured by Picker calorimeter (1971PIC/LED)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1988BOY/CRI	original data measured at 8.3 MPa converted to vapor pressure								
1988OKA/OGA	water content below 0.083 mol %								

Correlated heat capacities (42.2.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1968PAZ/REC	313.1	1	1.00	#	1.734	1.79−1	1.73	1.79−1	1
1971CAR/WES	180.0–320.0	17	0.10	#	0.122	1.12−3	0.01	−1.33−4	−2
1987LAN/CRI	298.1–313.1	2	0.50	#	0.282	1.38−2	0.14	−1.32−2	−2
1988BOY/CRI	393.1–503.1	5	3.00	#	1.016	5.99−1	3.05	1.66−1	1
1992FIL/AFA	298.1	1	1.00	#	2.069	1.98−1	2.07	−1.98−1	−1
1993CON/GIR1	298.0–343.2	5	5.00		0.644	3.39−1	3.22	3.30−1	5
1993NAZ/BAS	298.1–325.5	2	2.20		0.152	3.32−2	0.33	−3.22−2	−2
1997RIG/COM	308.1	1	1.00		1.584	1.61−1	1.58	1.61−1	1
2002PAR/ZOU	278.1–348.1	15	0.50	#	0.509	2.64−2	0.25	1.65−3	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1907WAL	(9.98−2, 1.03, 9.98−2, 1)	1925DRU/WEI	(1.96−1, 2.08, −1.96−1, −1)
1925PAR	(2.68−2, 0.29, 9.65−3, 4)	1929KEL1	(6.27−2, 0.73, −5.31−2, −12)
1929MIT/HAR1	(2.89−1, 3.14, 2.46−1, 16)	1931FIO/GIN	(1.25−1, 1.07, −1.15−1, −7)
1939PHI	(6.11−1, 5.86, 6.11−1, 1)	1949STA/GUP	(5.98−2, 0.69, −4.03−2, −4)
1949TSC/RIC2	(2.38−1, 2.38, 2.38−1, 1)	1950HOU/MAS2	(4.86−2, 0.45, 1.30−2, 2)
1960SWI/ZIE	(3.73−1, 3.84, −3.73−1, −1)	1962KAT	(6.92−1, 6.36, 6.76−1, 4)
1966DRA/LAN	(1.52−1, 1.53, 1.52−1, 1)	1971DES/BHA	(3.52−1, 3.38, 3.50−1, 3)
1971GOP/GAM	(7.04−1, 7.23, −6.90−1, −3)	1981ATA/ELS	(7.78−2, 0.80, 7.78−2, 1)
1982BEN/DAR	(5.69−2, 0.58, 8.53−3, 0)	1982VIL/CAS	(9.33−2, 0.95, 9.33−2, 1)
1984ZEG/SOM2	(3.91−2, 0.40, 3.91−2, 1)	1985COS/PAT8	(1.26−1, 1.27, −1.25−1, −2)
1986KOR/KUK	(5.98−2, 0.63, 5.27−2, 2)	1986OGA/MUR	(1.04−1, 1.08, −1.04−1, −1)
1986TAN/TOY	(5.00−2, 0.51, 5.00−2, 1)	1988AND/PAT	(1.09−1, 1.13, −1.09−1, −1)
1988OKA/OGA	(9.59−2, 0.99, −9.59−2, −2)	1989DOU/KHA	(7.98−3, 0.08, 7.98−3, 1)

Parameters of cubic spline polynomials (42.2.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−				
p	141	49	0.705	2.40−1	1.59	5.21−2	4				
Sat	141	49	0.818	3.70−1	1.94	5.52−2	7				
T/K			A_1		A_2		A_3		A_4		Uncert.
180.0–300.0			1.026 27+1		−1.463 11		2.476 15−2		1.372 99−1		II
300.0–400.0			4.604 47		4.195 11		−1.861 32		3.468 63−1		III
400.0–503.1			−4.061 88+2		3.122 89+2		−7.888 49+1		6.765 50		IV
180.0–300.0			1.056 00+1		−1.849 45		1.895 43−1		1.142 26−1		II
300.0–400.0			−1.686 34		1.039 68+1		−3.892 56		5.677 93−1		III
400.0–503.1			5.811 87+1		−3.445 69+1		7.320 89		−3.666 61−1		VI

Parameters of quasi-polynomial equation (42.2.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−						
p	141	49	2.938	2.85−1	1.59	−2.88−2	−23						
T/K		T_c/K		A_1		A_2		A_3	A_4	A_5		A_6	Uncert.
180.0–503.1		512.64		−2.835 12		3.683 44−2		7.806 67	3.978 00	−2.864 02+1		3.464 78+1	V

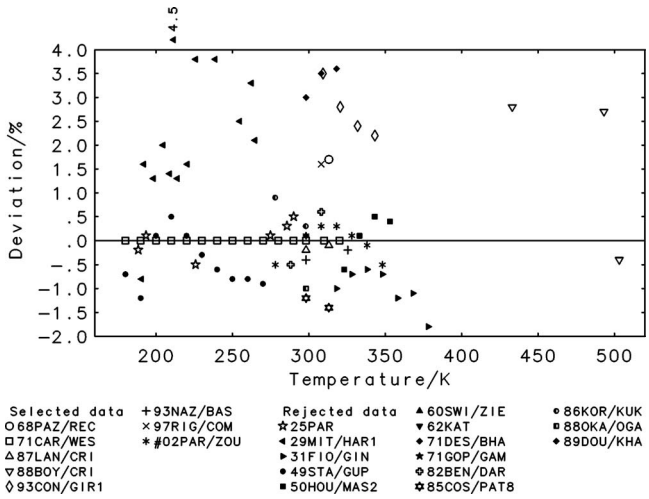

FIG. 77. Deviation plot for methanol (42-002).

Deviation plot for Methanol (42–002) is given in Fig. 77.

6.5.2.2. Ethanol (42-005)

Name:	Ethanol
Formula:	C_2H_6O
CAS-RN:	64-17-5
Group No:	42-005

Experimental heat capacities (42.5.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1907WAL		291.6	1		n/a	n/a	n/a	avg	DSIO	1907WAL
1920GIB/PAR		196.2–271.4	11		n/a	n/a	n/a	*p*	BSIO	1920GIB/LAT
1924WIL/DAN		300.0–332.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1925PAR	N	160.0–298.0	7	S	0.50	n/a	n/a	*p*	BSIO	1925PAR
1929KEL2		163.5–294.3	20		1.00	99.96	estim	*p*	BSIO	1929KEL1
1929MIT/HAR1		184.4–268.8	25		n/a	n/a	n/a	*p*	BSIO	1929MIT/HAR1
1931BLA/LEI		303.1–343.1	9		3.00	n/a	n/a	*p*	BSIO	1931BLA/LEI
1931FIO/GIN	N	318.1-378.1	7	S	0.10	n/a	n/a	sat	BSIO	1931FIO/GIN
1936ERN/WAT		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1939BYK		298.1	1		n/a	n/a	n/a	*p*	BSIT	1939BYK
1940MAZ		174.1–297.8	46		n/a	n/a	n/a	*p*	BSIO	1939MAZ3
1949TSC/RIC2		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1960SWI/ZIE	N	316.5	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1962RAB/NIK		288.1–328.1	9	S	0.30	n/a	n/a	*p*	BSAO	1947SKU
1965KAU/BIT		293.1–349.1	11		1.00	n/a	n/a	*p*	FSIO	1965KAU/BIT
1966HWA/ZIE		165.3–304.2	41		n/a	99.95	chrom	*p*	BSAO	1945SCO/MEY
1966KLE		293.1–343.1	11	S	0.10	n/a	n/a	*p*	BSAO	1966KLE
1967GRA		308.1–338.1	6		1.00	n/a	n/a	*p*	BSIO	1967GRA
1967NIK/RAB2		160.0–250.0	19	S	0.20	n/a	n/a	*p*	BSAO	1956POP/KOL
1968PAZ/REC	N	313.1	1		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1975PED/KAY		300.8–344.2	16		n/a	n/a	n/a	*p*	BSIO	1975PED/KAY
1976FOR/BEN1		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1976FOR/BEN2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1977HAI/SUG2		161.3–301.1	54		n/a	99.86	melpt	sat	BSAO	1965SUG/SEK

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1978BYV/JAS		293.1–333.1	3		2.00	n/a	n/a	*p*	BDCT	1978BYV/JAS
1979BRO/ZIE		159.0–306.0	eqn		n/a	99.94	melpt	*p*	BSAO	1945SCO/MEY
1982BEN/DAR		288.1–308.1	2		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1982VIL/CAS		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1984STE/OLS		266.1–318.1	11	S	n/a	n/a	n/a	*p*	BDHT	1969PER/COM
1984ZEG/SOM2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1985OGA		298.1	1		0.20	n/a	n/a	*p*	FSIO	1985OGA
1986KOR/KUK		298.0	1		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1986OGA/MUR		298.1	1		0.10	n/a	n/a	*p*	FSIO	1985OGA
1986TAN/TOY		298.1	1		0.30	99.96	anal	*p*	FSIT	1971PIC/LED
1988AND/PAT		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1989PET/PES1	N	258.1–318.1	4		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1994CON/GIA2		298.1	1		n/a	99.9	anal	*p*	FSIT	1988CON/GIA
1995CON/GIA1		91.0	1		0.50	99.9	chrom	*p*	FSIT	1988CON/GIA
1995CON/GIA2		298.1	1		n/a	99.9	anal	*p*	FSIT	1988CON/GIA
1995LOW/PEU		298.2	1		1.00	n/a	n/a	*p*	BDCO	1995LOW/PEU
1996TAN/TOY1		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
2004PEL/TRO		288.1–303.1	6		n/a	99.5	chrom	*p*	BDHT	1969PER/COM
2005PEL/TRO		283.1–303.1	5		n/a	99.5	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1925PAR	same data in 1927PAR/HUF
1931FIO/GIN	data calculated using procedure by 1985WIL/CHA
1960SWI/ZIE	average value in the temperature range 294–339 K
1968PAZ/REC	same datum in 1970PAZ/PAZ
1989PET/PES1	same data in 1990ALP/PES

Correlated heat capacities (42.5.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1931FIO/GIN	318.1–378.1	7	0.10		1.996	3.45−2	0.20	−7.16−3	−3
1940MAZ	174.1–297.9	46	1.00	#	1.218	1.57−1	1.22	6.07−2	−4
1966HWA/ZIE	165.3–304.2	41	1.00	#	0.255	2.85−2	0.26	1.55−2	11
1966KLE	293.1–343.1	11	0.10		1.238	1.79−2	0.12	−2.77−3	−3
1968PAZ/REC	313.1	1	1.00	#	0.041	5.80−3	0.04	5.80−3	1
1976FOR/BEN2	298.1	1	0.30		0.653	2.65−2	0.20	2.65−2	1
1977HAI/SUG2	163.1–301.1	53	1.00	#	0.272	3.04−2	0.27	1.59−2	16
1979BRO/ZIE	159.0–306.0	16	1.00	#	0.295	3.14−2	0.29	−5.18−3	−3
1986OGA/MUR	298.1	1	0.10		2.137	2.89−2	0.21	2.89−2	1
1989PET/PES1	258.1–318.1	4	0.20		0.770	2.10−2	0.15	1.64−2	2
1994CON/GIA2	298.1	1	1.00	#	0.232	3.13−2	0.23	−3.13−2	−1
1995CON/GIA1	91.0	1	0.50		0.053	3.53−3	0.03	3.53−3	1
1995CON/GIA2	298.1	1	1.00	#	0.188	2.52−2	0.19	−2.52−2	−1
1995LOW/PEU	298.2	1	1.00		0.253	3.42−2	0.25	3.42−2	1
1996TAN/TOY1	298.1	1	0.50	#	0.321	2.17−2	0.16	2.17−2	1
2004PEL/TRO	288.1–303.1	6	0.50	#	0.234	1.57−2	0.12	−1.56−2	−6
2005PEL/TRO	283.1–303.1	5	0.50	#	0.237	1.56−2	0.12	−1.54−2	−5

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1907WAL	(1.89−1, 1.41, 1.89−1, 1)	1920GIB/PAR	(1.26−1, 1.18, −1.01−1, −9)
1924WIL/DAN	(4.58−1, 2.96, 4.00−1, 8)	1925PAR	(9.27−2, 0.73, 4.78−2, 1)
1929KEL2	(7.74−2, 0.69, −3.44−2, −8)	1929MIT/HAR1	(5.42−1, 4.53, 5.25−1, 25)
1931BLA/LEI	(7.83−1, 4.77, 7.02−1, 9)	1936ERN/WAT	(1.06, 8.52, −1.06, −1)
1939BYK	(3.89−2, 0.29, −3.89−2, −1)	1949TSC/RIC2	(4.71−1, 3.38, 4.71−1, 1)
1960SWI/ZIE	(1.35−1, 0.94, −1.35−1, −1)	1962RAB/NIK	(8.81−2, 0.62, 4.84−2, 5)
1965KAU/BIT	(1.44−1, 1.01, 2.16−2, 5)	1967GRA	(8.08−2, 0.56, −4.16−2, −2)
1967NIK/RAB2	(6.76−2, 0.64, −4.92−2, −19)	1975PED/KAY	(2.37−1, 1.52, 2.04−1, 14)
1976FOR/BEN1	(3.11−3, 0.02, −3.11−3, −1)	1978BYV/JAS	(6.22−1, 4.34, −3.26−1, −1)
1982BEN/DAR	(1.28−1, 0.91, 6.96−2, 0)	1982VIL/CAS	(1.96−1, 1.43, 1.96−1, 1)
1984STE/OLS	(4.13−1, 2.96, 4.05−1, 11)	1984ZEG/SOM2	(6.62−2, 0.49, 6.62−2, 1)
1985OGA	(1.94−1, 1.46, −1.94−1, −1)	1986KOR/KUK	(8.89−2, 0.66, 8.89−2, 1)
1986TAN/TOY	(6.74−2, 0.50, 6.74−2, 1)	1988AND/PAT	(7.09−2, 0.53, −7.09−2, −1)

Parameters of cubic spline polynomials (42.5.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	367	197	0.823	8.11−2	0.64	2.06−2	9
sat	367	197	0.822	8.10−2	0.64	2.06−2	8

T/K	A_1	A_2	A_3	A_4	Uncert.
91.0–220.0	2.703 90+1	−2.352 44+1	1.06680+1	−1.485 31	II
220.0–290.0	2.076 58	1.051 52+1	−4.804 53	8.590 18−1	I
290.0–378.2	3.543 40+1	−2.399 25+1	7.09467	−5.087 05−1	II
91.0–220.0	2.703 21+1	−2.351 02+1	1.06591+1	−1.483 53	II
220.0–290.0	2.137 53	1.043 70+1	−4.771 49	8.544 34−1	I
290.0–378.2	3.662 41+1	−2.523 88+1	7.530 50	−5.595 86−1	II

Parameters of quasipolynomial equation (42.5.4)

type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	367	196	0.928	7.50−2	0.59	5.01−3	−17

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
159.0–378.1	513.92	1.615 30+1	3.922 68−1	9.342 74	2.615 21+1	−4.023 80+1	8.000 67+1	III

Deviation plot forEthanol (42–005) is given in Fig. 78.

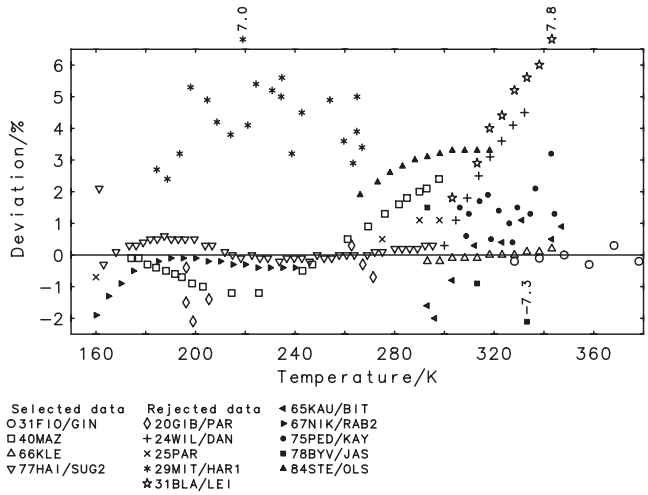

FIG. 78. Deviation plot for ethanol (42-005).

6.5.2.3. 1,2-Ethanediol (42-006)

Name:	1,2-Ethanediol
Formula:	$C_2H_6O_2$
CAS-RN:	107-21-1
Group No:	42-006

Experimental heat capacities (42.6.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	378.1–382.1	2		n/a	n/a	n/a	avg	DSIO	1898LOU
1901DEF	N	309.4–349.1	2		n/a	n/a	n/a	avg	n/a	n/a
1902LOU1	N	380.6	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1909SCH		295.1–308.1	2		n/a	n/a	n/a	*p*	BSIO	1909SCH
1925PAR/KEL	N	262.0–293.0	6		n/a	99.	estim	*p*	BSIO	1925PAR
1932NEU/KUR		293.4–351.5	3		n/a	n/a	n/a	*p*	BSIO	1932NEU
1957CRU/JOS		293.1–338.1	2		2.00	n/a	n/a	*p*	BSIO	1957CRU/JOS
1962RAB/NIK		283.1–328.1	10	S	0.30	n/a	n/a	*p*	BSAO	1947SKU
1965TUN/MIS		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1967NIK/RAB1		265.0–310.0	10	S	n/a	n/a	n/a	*p*	BSAO	1956POP/KOL
1968PAZ/REC	N	301.1–313.1	2		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1972KAW/OTA		303.1	1		1.00	n/a	n/a	*p*	BSIO	1949WEI
1976NIC/SKO		298.1	1		0.20	n/a	n/a	*p*	DDCT	1971KON/SUU
1977MUR/SUB		298.1	1		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1979STE/TAM		273.1–493.1	15	S	n/a	99.9	chrom	sat	BDHT	1969PER/COM
1982ZAR		298.0–363.0	3		0.60	99.7	chrom	*p*	BDCT	1982ZAR
1988MUK/ZAR		298.7–433.3	6		n/a	n/a	n/a	*p*	BDCT	1982ZAR
1991DOU/PAL		298.1	1		n/a	99.5	estim	*p*	FSIT	1971PIC/LED
1999TAK/YAM		260.8–300.3	16		n/a	n/a	n/a	*p*	BSAO	1987YAM/OGU
2002NAN/LIU		273.1–373.1	21		0.50	n/a	n/a	*p*	BSAO	1995TAN/SUN
2003YAN/MA1		293.1–373.1	11		1.00	99.8	chrom	*p*	BDHT	2003YAN/MA1
2003YAN/MA2		293.1–373.1	17		2.00	n/a	n/a	*p*	BDHT	2004YAN/MA

Reference	Notes
1898LOU	average values in the temperature ranges 295–461 and 296–468 K
1901DEF	average values in the temperature ranges 286–412 and 286–333 K; calorimeter not identified, probably drop

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1902LOU1	average value in the temperature range 293–468 K								
1925PAR/KEL	original values decreased by 1.5 %—correction for water content, recommendation given in 1985WIL/CHA								
1968PAZ/REC	same data in 1970PAZ/PAZ								

Correlated heat capacities (42.6.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1898LOU	378.1–382.1	2	3.00	#	0.545	3.37−1	1.64	−3.37−1	−2
1901DEF	309.5–349.1	2	3.00	#	0.273	1.60−1	0.82	−1.33−1	−2
1902LOU1	380.6	1	3.00	#	0.489	3.12−1	1.47	3.12−1	1
1909SCH	295.1–308.1	2	3.00	#	0.298	1.63−1	0.89	4.13−2	0
1925PAR/KEL	262.0–293.0	6	1.00	#	0.229	3.95−2	0.23	2.15−2	2
1932NEU/KUR	293.4–351.5	3	3.00	#	0.443	2.52−1	1.33	−2.39−1	−3
1968PAZ/REC	301.1–313.1	2	0.70	#	0.933	1.19−1	0.65	−1.85−3	0
1979STE/TAM	273.1–493.1	15	1.00	#	0.350	7.10−2	0.35	3.79−2	5
1982ZAR	298.0–363.0	3	0.60		1.502	1.76−1	0.90	−1.28−2	1
1988MUK/ZAR	298.7–433.3	6	1.00	#	0.992	1.94−1	0.99	−1.17−1	−2
1999TAK/YAM	260.8–300.3	16	1.00	#	1.165	2.00−1	1.16	1.96−1	16
2002NAN/LIU	273.1–373.1	21	0.50		1.187	1.03−1	0.59	−2.02−2	5
2003YAN/MA1	293.1–373.1	11	2.00	#	0.850	3.29−1	1.70	−2.51−1	−7
2003YAN/MA2	293.1–373.1	17	2.00		0.147	5.71−2	0.29	−4.76−2	−13

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1957CRU/JOS	(4.97, 18.83, 3.43, 0)	1962RAB/NIK	(8.89−2, 0.47, 7.11−2, 10)
1965TUN/MIS	(1.69−1, 0.95, −1.69−1, −1)	1967NIK/RAB1	(1.97−1, 1.10, 1.90−1, 10)
1972KAW/OTA	(6.16−1, 3.53, −6.16−1, −1)	1977MUR/SUB	(1.14−1, 0.63, 1.14−1, 1)
1991DOU/PAL	(1.40−1, 0.79, −1.40−1, −1)		

Parameters of regression polynomial (42.6.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	133	107	0.866	1.74−1	0.93	−2.03−2	1
sat	133	107	0.866	1.75−1	0.93	−2.03−2	1

T/K	A_1	A_2	A_3	A_4	Uncert.
260.8–493.1	5.317 03	4.595 25	−1.281 51−1		IV
260.8–493.1	5.263 96	4.628 84	−1.334 07−1		IV

Parameters of quasipolynomial equation (42.6.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	133	107	1.035	1.61−1	0.84	1.63−2	25

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
260.8–493.1	790.00	−7.444 44−1	4.780 44−3	7.804 53	2.502 64+1	1.8811 52	4.705 43−2	IV

Deviation plot for 1,2–Ethanediol (42–006) is given in Fig. 79.

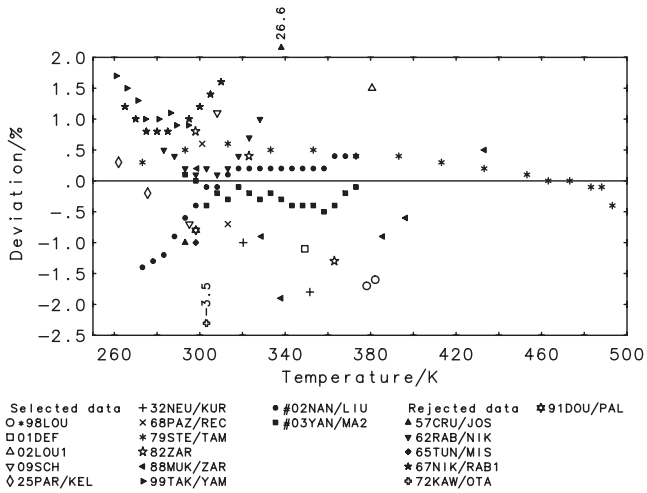

FIG. 79. Deviation plot for 1,2-ethanediol (42-006).

6.5.2.4. 1-Propanol (42-009)

Name:	1-Propanol
Formula:	C_3H_8O
CAS-RN:	71-23-8
Group No:	42-009

Experimental heat capacities (42.9.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1920GIB/PAR		165.7–274.6	29		n/a	n/a	n/a	*p*	BSIO	1920GIB/LAT
1926PAR/HUF	N	152.1–275.0	7		n/a	n/a	n/a	*p*	BSIO	1925PAR
1927PAR/HUF		169.1–275.3	7		n/a	n/a	n/a	*p*	BSIO	1925PAR
1929MIT/HAR1		162.8–274.4	35		n/a	n/a	n/a	*p*	BSIO	1929MIT/HAR1
1939PHI		301.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1941ZHD		279.6–318.8	5		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1949TSC/RIC2		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1951EUC/EIG		273.0–393.0	12	S	n/a	n/a	n/a	sat	BSAO	1951EUC/EIG
1960SWI/ZIE	N	320.9	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1968COU/LEE		153.9–361.5	47		0.10	99.75	melpt	*p*	BSAO	1963AND/COU1
1968PAZ/REC	N	313.1	1		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1968REC1	N	298.0–313.0	eqn		n/a	n/a	n/a	*p*	BSAO	1968REC1
1976FOR/BEN1		298.1–298.1	2		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1976FOR/BEN2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1977MUR/SUB		298.1	1		0.30	n/a	n/a	*p*	BSIO	1964MOE/THO
1979GRI/YAN	N	303.4–463.0	11		0.90	n/a	n/a	*p*	BDAO	1975RAS/GRI
1980KAL/JED		181.8–303.1	66		0.20	99.95	chrom	*p*	BSAO	1980KAL/JED
1981ARU/BAG		293.1–353.1	4	S	1.50	99.0	melpt	*p*	BDHT	1981ARU
1982BEN/DAR		288.1–308.1	2	S	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1982VIL/CAS		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1984ZEG/SOM2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986KOR/KUK		278.0–298.0	2		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1986TAN/TOY		298.1	1		0.30	99.9	anal	*p*	FSIT	1971PIC/LED
1991OGA/MIT		298.1	1		n/a	n/a	n/a	*p*	FSIO	1985OGA
1995LOW/PEU		298.2	1		1.00	n/a	n/a	*p*	BDCO	1995LOW/PEU
1997HOV/ROU		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1999CER/TOV		288.1–308.1	4	n/a	99.5	chrom	*p*	BDCT	1983ROU/ROU
2000BEC/AUF	N	307.0–337.0	7	0.30	99.95	chrom	sat	BDCT	2000BEC/AUF
2000BEC/AUF	N	330.1–354.9	6	0.20	99.95	chrom	sat	BDCT	2000BEC/AUF
2001PEL/GON		280.1–318.1	5	n/a	99.5	chrom	*p*	BDHT	1969PER/COM
2002PEL/GON		280.1–318.1	5	n/a	99.8	chrom	*p*	BDHT	1969PER/COM
2004FEN/PER		298.1	1	n/a	99.0	anal	*p*	FSIT	1971PIC/LED
2004VAN/VAN		153.0–350.0	81	0.20	99.94	melpt	*p*	BSAO	1987VAN/VAN

Reference	Notes
1926PAR/HUF	high sample purity
1960SWI/ZIE	average value in the temperature range 294–347 K
1968PAZ/REC	same datum in 1970PAZ/PAZ
1968REC1	same data in 1968REC2 and 1968REC3
1979GRI/YAN	data above 343.28 K measured at elevated pressures up to 1.52 MPa
2000BEC/AUF	step by step method was used
2000BEC/AUF	three-step method was used

6.5.2.5. 2-Propanol (42-010)

Name:	2-Propanol
Formula:	C_3H_8O
CAS-RN:	67-63-0
Group No:	42-010

Experimental heat capacities (42.10.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1924WIL/DAN		303.0–28.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1925PAR/KEL		195.4–93.1	9		n/a	n/a	n/a	*p*	BSIO	1925PAR
1928PAR/KEL	N	195.4–93.1	11		1.00	99.96	estim	*p*	BSIO	1925PAR
1929KEL3		188.4–92.8	12		1.00	99.95	estim	*p*	BSIO	1929KEL1
1933TRE/WAT		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1939PHI		303.1	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1945ZHD		280.0–20.0	4		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1948GIN/COR		273.1–73.1	11	S	n/a	n/a	n/a	sat	DSTO	1950GIN/DOU
1958SWI/ZIE2	N	324.0	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1962KAT		293.1–43.1	3		n/a	n/a	n/a	*p*	BSIO	1962KAT
1963AND/COU2		188.3–27.1	60		n/a	n/a	n/a	*p*	BSAO	1963AND/COU1
1977HOF/SAN	N	353.1–63.1	12	S	1.00	n/a	n/a	*p*	FSIO	1975SAN
1979BRO/ZIE		185.0–04.0	eqn		n/a	99.84	melpt	*p*	BSAO	1945SCO/MEY
1979GRI/YAN		329.3–41.5	2		0.90	n/a	n/a	*p*	BDAO	1975RAS/GRI
1980ROU/ROB		283.1–98.1	2		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986KOR/KUK		298.0	1		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1993CON/GIR1		298.0–63.0	eqn		5.00	n/a	n/a	sat	BDHT	1993CON/GIR1
1993NAZ/BAS		302.4–49.0	3		2.20	99.6	anal	*p*	BDHO	1986NAZ/BAS1
1995LOW/PEU		298.2	1		1.00	n/a	n/a	*p*	BDCO	1995LOW/PEU
1996TAN/TOY2		298.1	1		n/a	99.98	chrom	*p*	FSIT	1971PIC/LED
1999CER/TOV		288.1–08.1	4		n/a	99.9	chrom	*p*	BDCT	1983ROU/ROU
2004FEN/PER		298.1	1		1.00	99.0	anal	*p*	FSIT	1971PIC/LED

Reference	Notes
1928PAR/KEL	similar data in 1925PAR/KEL

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1958SWI/ZIE2	average value in the erature range 294–354 K								
1977HOF/SAN	C_p at saturation curve extrapolated from high pressure measurements								

Correlated heat capacities (42.10.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/-
1948GIN/COR	273.1–73.1	11	0.80	#	0.940	1.75–1	0.75	−6.25–2	−3
1963AND/COU2	188.3–27.1	60	0.20	#	1.214	4.52–2	0.24	1.78–3	−3
1979BRO/ZIE	185.0–03.8	13	0.30	#	0.791	3.72–2	0.24	−1.07–2	−3
1979GRI/YAN	329.3–41.5	2	0.90		0.412	8.17–2	0.37	3.57–2	0
1993NAZ/BAS	302.4–49.0	3	2.20		1.039	5.06–1	2.29	5.01–1	3
1995LOW/PEU	298.2	1	1.00		0.468	8.69–2	0.47	−8.69–2	−1
1996TAN/TOY2	298.1	1	0.50	#	0.299	2.78–2	0.15	−2.78–2	−1
1999CER/TOV	288.1–08.1	4	1.00	#	0.414	7.74–2	0.41	7.70–2	4
2004FEN/PER	298.1	1	1.00		0.025	4.65–3	0.02	4.65–3	1

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1924WIL/DAN	(1.47, 6.70, 1.47, 3)	1925PAR/KEL	(9.97–2, 0.64, 9.11–2, 7)
1928PAR/KEL	(7.35–2, 0.50, 2.30–2, 3)	1929KEL3	(2.27–1, 1.50, −2.03–1, −12)
1933TRE/WAT	(9.95–1, 5.06, 9.95–1, 1)	1939PHI	(1.60, 7.73, 1.60, 1)
1945ZHD	(6.70–1, 3.25, 6.11–1, 4)	1958SWI/ZIE2	(4.70–1, 2.16, 4.70–1, 1)
1962KAT	(8.24–1, 3.99, 7.96–1, 3)	1977HOF/SAN	(7.83–1, 2.74, 7.47–1, 12)
1980ROU/ROB	(5.28–1, 2.74, 4.49–1, 2)	1986KOR/KUK	(1.03–1, 0.55, 1.03–1, 1)
1993CON/GIR1	(1.88, 9.23, −1.85, −6)		

Parameters of cubic spline polynomials (42.10.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	162	96	1.110	1.20–1	0.55	1.10–2	−3
sat	162	96	1.107	1.20–1	0.55	1.02–2	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
185.0–270.0	−1.124 27+1	3.274 59+1	−1.550 78+1	2.651 21	II
270.0–360.0	1.122 66+2	−1.044 86+2	3.531 90+1	−3.623 70	IV
360.0–473.2	−1.755 13+2	1.353 30+2	−3.129 66+1	2.544 40	V
185.0–270.0	−1.1096 7+1	3.255 85+1	−1.542 86+1	2.640 20	II
270.0–360.0	1.122 91+2	−1.045 39+2	3.534 82+1	−3.628 54	IV
360.0–473.2	−1.266 06+2	9.454 15+1	−1.995 19+1	1.491 84	V

Parameters of quaspolynomial equation (42.10.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	162	96	2.045	3.13–1	1.16	−2.97–2	−7

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
185.0–473.1	508.30	1.540 26+2	8.485 17	2.805 94−1	1.946 54+2	−1.250 38+2	3.107 63+2	V

Deviation plot for 2–Propanol (42–010) is given in Fig. 80.

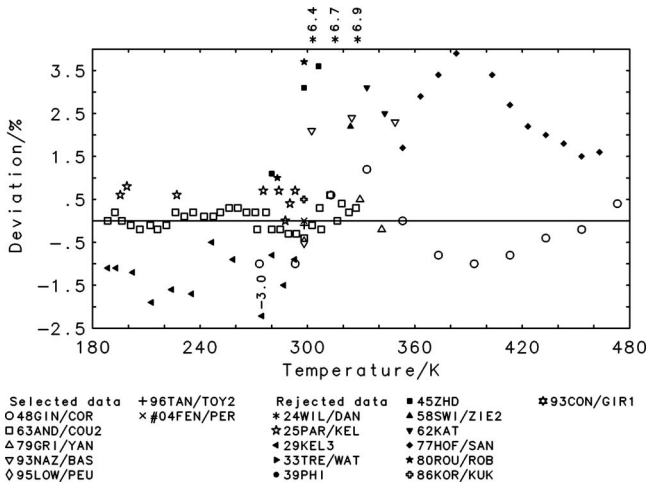

FIG. 80. Deviation plot for 2-propanol (42-010).

6.5.2.6. 1,2-Propanediol (42-011)

Name:	1,2-Propanediol
Formula:	$C_3H_8O_2$
CAS-RN:	57-55-6
Group No:	42-011

Experimental heat capacities (42.11.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1927PAR/HUF		194.3–276.6	7		n/a	n/a	n/a	*p*	BSIO	1925PAR
1952CUR/JOH	N	213.1–460.5	26	S	n/a	n/a	n/a	sat	n/a	n/a
1972KAW/OTA		303.1	1		1.00	n/a	n/a	*p*	BSIO	1949WEI
1982ZAR		298.0–363.0	3		0.60	99.87	chrom	*p*	BDCT	1982ZAR
2002STE/CHI3		300.0–600.0	16	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2003YAN/MA2		293.1–363.1	15		2.00	n/a	n/a	*p*	BDHT	2004YAN/MA

Reference	Notes
1952CUR/JOH	correlated data [sources: Dow Chemical Co. (technical product) and 1927PAR/HUF]

Correlated heat capacities (42.11.2)

Reference	*T*/K	nPts	$\sigma_r C$/%		d_w	*d*/R	d_r/%	d_b/R	+/−
1927PAR/HUF	194.3–276.6	7	1.00	#	0.215	4.43−2	0.21	2.53−2	5
1952CUR/JOH	213.1–423.1	22	3.00	#	0.294	2.33−1	0.88	1.18−1	16
1982ZAR	298.0–363.0	3	0.60		0.652	1.01−1	0.39	1.73−2	−1
2002STE/CHI3	300.0–600.0	16	1.00		0.310	9.23−2	0.31	2.10−3	4
2003YAN/MA2	293.1–348.1	12	2.00		0.563	2.78−1	1.13	−1.99−1	−8

Rejected data: Reference (*d*/R, d_r, d_b/R, +/-)

1972KAW/OTA	(1.54, 7.15, −1.54, −1)

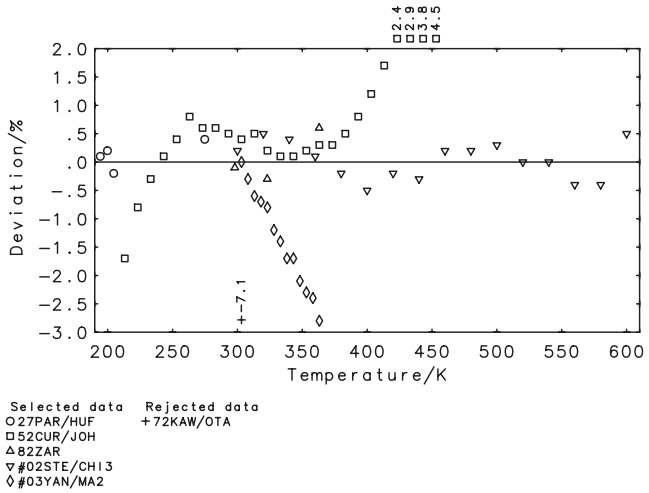

FIG. 81. Deviation plot for 1,2-propanediol (42-011).

Parameters of cubic spline polynomials (42.11.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	68	60	0.401	2.05−1	0.79	7.99−3	16
sat	68	60	0.393	2.02−1	0.79	7.92−3	16

T/K	A_1	A_2	A_3	A_4	Uncert.
194.3–400.0	2.706 94+1	−1.446 89+1	6.417 52	−6.835 42−1	II
400.0–600.0	−5.976 18+1	5.065 45+1	−9.863 33	6.731 95−1	III
194.3–400.0	2.662 69+1	−1.399 80+1	6.257 44	−6.660 87−1	II
400.0–600.0	−5.149 15+1	4.459 09+1	−8.389 76	5.545 13−1	III

Parameters of quasi-polynomial equation (42.11.4)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	68	60	0.891	2.94−1	1.04	2.77−2	20

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
194.3–600.0	676.40	1.367 35+2	1.176 80+1	1.755 94	1.310 62+2	8.276 85+1	6.561 73+1	IV

Deviation plot for 1,2–Propanediol (42–011) is given in Fig. 81.

6.5.2.7. 1-Butanol (42-013)

Name:	1-Butanol
Formula:	$C_4H_{10}O$
CAS-RN:	71-36-3
Group No:	42-013

Experimental heat capacities (42.13.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1924WIL/DAN		303.0–348.0	eqn	n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1925PAR		194.6–294.0	12	0.50	n/a	n/a	p	BSIO	1925PAR
1933TRE/WAT		298.1	1	n/a	n/a	n/a	p	BSIO	1949WEI
1938PAN/DUD	N	298.0–363.0	eqn	n/a	n/a	n/a	p	n/a	n/a

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1939PHI		302.5	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1949TSC/RIC2		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1960SWI/ZIE	N	322.4	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1965COU/HAL		188.2–322.3	25		0.20	99.94	melpt	*p*	BSAO	1963AND/COU1
1967GRA		308.1–338.1	4		1.00	n/a	n/a	*p*	BSIO	1967GRA
1968PAZ/REC	N	301.1–313.1	2		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1975SAN	N	295.9–466.6	20		0.90	n/a	n/a	*p*	FSIO	1975SAN
1978BYV/JAS		293.1–333.1	3		2.00	n/a	n/a	*p*	BDCT	1978BYV/JAS
1979GRI/YAN	N	324.0–462.5	8	S	0.90	n/a	n/a	*p*	BDAO	1975RAS/GRI
1981ARU/BAG		293.1–373.1	5	S	1.50	n/a	n/a	*p*	BDHT	1981ARU
1986GAT/WOO		298.1–368.1	4		n/a	99.	anal	*p*	BDCT	1983ROU/ROU
1986KOR/KUK		278.0–298.0	2		0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1986NAZ/BAS1		321.0–373.4	3		2.00	n/a	n/a	*p*	BDHO	1986NAZ/BAS1
1986OGA/MUR		298.1	1		0.10	n/a	n/a	*p*	FSIO	1985OGA
1986ROU/GRO		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1986TAN/TOY		298.1	1		0.30	99.9	anal	*p*	FSIT	1971PIC/LED
1988AND/PAT		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1988PIE/SOM2		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1989COB/GAR		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1997HOV/ROU		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1999CAL/BRO		298.1	1		n/a	99.8	chrom	*p*	FSIT	1971PIC/LED
2001CER/TOV1		288.1–308.1	4		n/a	99.8	chrom	*p*	BDHT	1969PER/COM
2002PAR/ZOU		278.1–348.1	15		n/a	99.5	chrom	sat	BDCT	1983ROU/ROU
2004FEN/PER		298.1	1		1.00	99.0	anal	*p*	FSIT	1971PIC/LED
2005ZOR/CHO		285.1–353.1	28		n/a	99.5	chrom	*p*	BDCT	2000ERN/CHO

Reference	Notes
1938PAN/DUD	temperature range of parameters validity estimated by the compilers
1960SWI/ZIE	average value in the temperature range 294–350 K
1968PAZ/REC	same data in 1970PAZ/PAZ; apparently wrong value at 313.15 K
1975SAN	C_p at pressure near 1.4 MPa
1979GRI/YAN	data above 363.61 K measured at elevated pressures up to 0.92 MPa

Correlated heat capacities (42.13.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1965COU/HAL	188.2–322.3	25	0.20		0.988	4.27−2	0.20	9.59−3	3
1975SAN	295.9–466.6	20	0.90		1.200	3.18−1	1.08	−3.95−2	−2
1979GRI/YAN	324.0–462.5	8	0.90		1.173	3.47−1	1.05	1.62−1	0
1986GAT/WOO	298.1–368.1	4	0.40	#	0.825	8.57−2	0.33	−8.12−2	−4
1986OGA/MUR	298.1	1	0.10		0.915	1.95−2	0.09	1.95−2	1
1986TAN/TOY	298.1	1	0.30		0.618	3.94−2	0.19	−3.94−2	−1
1988AND/PAT	298.1	1	0.30	#	0.298	1.90−2	0.09	−1.90−2	−1
1988PIE/SOM2	298.1	1	0.30	#	0.117	7.48−3	0.04	7.48−3	1
1997HOV/ROU	298.1	1	1.00	#	0.282	5.99−2	0.28	−5.99−2	−1
1999CAL/BRO	298.1	1	1.00	#	0.305	6.47−2	0.30	−6.47−2	−1
2001CER/TOV1	288.1–308.1	4	0.20	#	0.339	1.46−2	0.07	1.40−2	4
2002PAR/ZOU	278.1–348.1	15	0.30	#	0.779	5.20−2	0.23	−9.99−3	−3
2004FEN/PER	298.1	1	1.00		0.046	9.88−3	0.05	9.88−3	1
2005ZOR/CHO	285.1–353.1	28	0.20	#	0.337	1.58−2	0.07	−7.45−3	−15

Rejected data: Reference	$(d/\mathrm{R}, d_r, d_b/\mathrm{R}, +/-)$		
1924WIL/DAN	(8.44−2, 0.35, 4.40−2, 3)	1925PAR	(8.14−2, 0.40, 3.35−2, 4)
1933TRE/WAT	(7.54−1, 3.42, 7.54−1, 1)	1938PAN/DUD	(1.37, 5.68, 1.06, 4)
1939PHI	(4.26, 16.44, 4.26, 1)	1949TSC/RIC2	(9.03−1, 4.07, 9.03−1, 1)
1960SWI/ZIE	(7.87−1, 3.46, −7.87−1, −1)	1967GRA	(2.57−1, 1.09, −2.26−1, −4)
1968PAZ/REC	(1.47, 7.14, −1.01, 0)	1978BYV/JAS	(2.13, 10.00, −1.82, −3)
1981ARU/BAG	(4.05−1, 1.59, −3.42−1, −3)	1986KOR/KUK	(1.10−1, 0.54, 1.09−1, 2)
1986NAZ/BAS1	(9.48−1, 3.58, −8.53−1, −3)	1986ROU/GRO	(1.26−1, 0.60, −1.26−1, −1)
1989COB/GAR	(2.26−1, 1.07, −2.26−1, −1)		

Parameters of cubic spline polynomials (42.13.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	159	111	0.879	1.72−1	0.58	−2.19−4	−18
sat	159	111	0.880	1.72−1	0.58	−4.02−4	−18

T/K	A_1	A_2	A_3	A_4	Uncert.
188.2–310.0	1.450 02+1	2.954 83	−2.45 761	7.480 81−1	II
310.0–390.0	1.839 00+2	−1.609 80+2	5.042 46+1	−4.938 18	III
390.0–466.6	−4.376 28+2	3.171 18+2	−7.216 46+1	5.539 53	V
188.2–310.0	1.446 86+1	2.994 06	−2.473 63	7.502 32−1	II
310.0–390.0	1.854 81+2	−1.625 02+2	5.091 22+1	−4.990 18	III
390.0–466.6	−4.247 62+2	3.069 16+2	−6.945 14+1	5.297 30	V

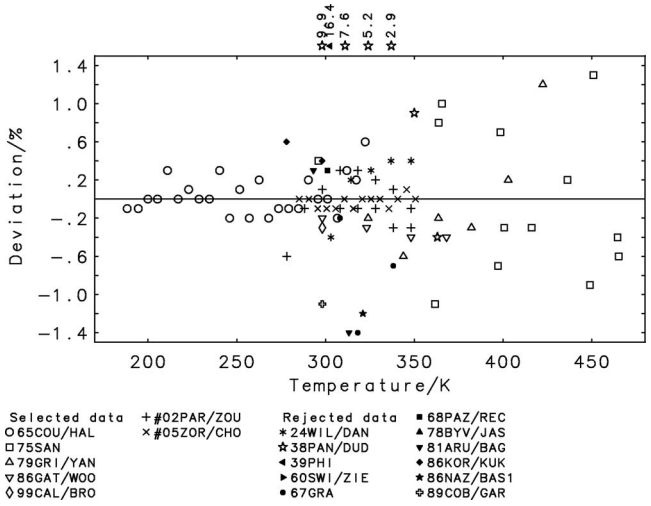

FIG. 82. Deviation plot for 1-butanol (42-013).

Parameters of quasipolynomial equation (42.13.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	159	111	1.850	2.39−1	0.81	−1.70−2	−21

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
188.2–466.6	563.05	4.080 39+2	3.054 01+1	−1.892 22+1	4.35783+2	−8.226 92+1	5.076 74+2	V

Deviation plot for 1–Butanol (42–013) is given in Fig. 82.

6.5.2.8. 2-Butanol (42-014)

Name:	2-Butanol
Formula:	$C_4H_{10}O$
CAS-RN:	78-92-2
Group No:	42-014

Experimental heat capacities (42.14.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1938PAN/DUD	N	298.0–363.0	eqn	n/a	n/a	n/a	*p*	n/a	n/a
1976CON/GIA		298.1	1	n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1988OKA/OGA	N	298.1	1	n/a	n/a	n/a	*p*	FSIO	1985OGA
1996TAN/TOY2		298.1	1	n/a	99.94	chrom	*p*	FSIT	1971PIC/LED
2000CER/MIG	N	288.1–308.1	4	n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2000CER/MIG	N	288.1–308.1	4	n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2004FEN/PER		298.1	1	1.00	99.0	anal	*p*	FSIT	1971PIC/LED
2004TRO/VAL		288.1–318.1	4	n/a	99.45	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1938PAN/DUD	temperature range of parameters validity estimated by the compilers
1988OKA/OGA	water content below 0.083 mol.%
2000CER/MIG	Scanning method
2000CER/MIG	Isothermal step method

Correlated heat capacities (42.14.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1976CON/GIA	298.1	1	1.00	#	1.197	2.87−1	1.20	2.87−1	1
1988OKA/OGA	298.1	1	1.00	#	0.635	1.51−1	0.63	1.51−1	1
1996TAN/TOY2	298.1	1	1.00	#	0.282	6.69−2	0.28	6.69−2	1
2000CER/MIG	288.1–308.1	4	1.00	#	0.390	8.83−2	0.39	−7.97−2	−4
2000CER/MIG	288.1–308.1	4	1.00	#	0.420	9.51−2	0.42	−8.69−2	−4
2004FEN/PER	298.1	1	1.00		0.519	1.23−1	0.52	1.23−1	1
2004TRO/VAL	288.1–318.1	4	1.00	#	0.391	9.29−2	0.39	1.38−2	0

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1938PAN/DUD	(1.74, 6.71, 1.71, 2)

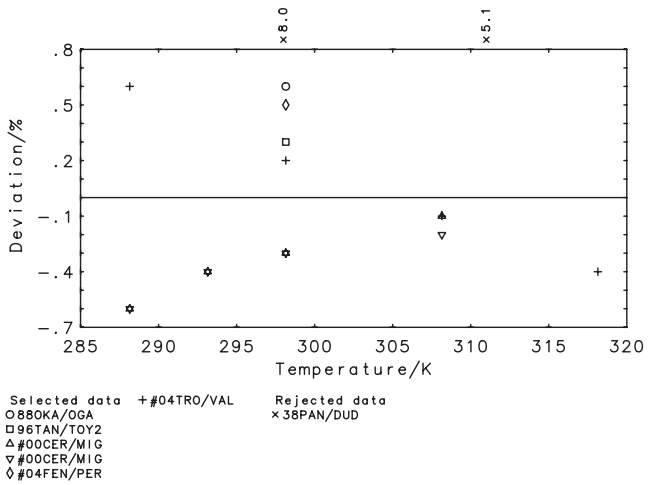

FIG. 83. Deviation plot for 2-butanol (42-014).

Parameters of regression polynomial (42.14.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	22	16	0.542	1.27−1	0.54	1.08−3	−4

T/K	A_1	A_2	A_3	A_4	Uncert.
288.1–318.1	−1.559 15+1	1.316 71+1	III		

Deviation plot for 2–Butanol (42–014) is given in Fig. 83.

6.5.2.9. 2-Methyl-1-propanol (42-017)

Name:	2-Methyl-1-propanol
Formula:	$C_4H_{10}O$
CAS-RN:	78-83-1
Group No:	42-017

Experimental heat capacities (42.17.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		308.6–328.1	9	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1898LOU	N	337.9	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1924WIL/DAN		303.0–353.0	eqn		n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1941ZHD		278.3–319.0	3		n/a	n/a	n/a	p	BSIT	1934KOL/UDO2
1958SWI/ZIE2	N	333.6–336.7	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1960SWI/ZIE	N	322.6	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1968COU/LEE		180.0–355.0	65		0.15	99.96	melpt	p	BSAO	1963AND/COU1
1968PAZ/REC	N	301.1–313.1	2		n/a	n/a	n/a	p	BDCT	1970PAZ/PAZ
1977HOF/SAN	N	383.1–493.1	12	S	1.00	n/a	n/a	p	FSIO	1975SAN
1978RYB/EME		293.1–353.1	7	S	n/a	n/a	n/a	p	BSIO	1978RYB/EME
1986KOR/KUK		298.0	1		0.20	n/a	n/a	p	BSAO	1983KUK/KOR
1988OKA/OGA	N	298.1	1		n/a	n/a	n/a	p	FSIO	1985OGA
1988PIE/SOM1		298.1	1		n/a	99.5	chrom	p	FSIT	1971PIC/LED
1992NAZ/BAS		300.6–396.1	5		2.20	99.8	chrom	p	BDHO	1986NAZ/BAS1
1997HOV/ROU		298.1	1		n/a	99.5	chrom	p	FSIT	1971PIC/LED
2000BEC/AUF	N	307.0–332.0	6		0.30	99.95	chrom	sat	BDCT	2000BEC/AUF

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000BEC/AUF	N	323.2–363.2	9	0.20	99.95	chrom	sat	BDCT	2000BEC/AUF
2000CER/MIG	N	288.1–308.1	4	n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2000CER/MIG	N	288.1–308.1	4	n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2004FEN/PER		298.1	1	1.00	99.0	anal	*p*	FSIT	1971PIC/LED

Reference	Notes
1898LOU	average value in temperature range 294–382 K
1958SWI/ZIE2	average values in temperature ranges 295–372 K and 295–379 K
1960SWI/ZIE	average value in temperature range 294–351 K
1968PAZ/REC	same data in 1970PAZ/PAZ
1977HOF/SAN	C_p at saturation curve extrapolated from high pressure measurements
1988OKA/OGA	water content below 0.083 mol.%
2000BEC/AUF	"step by step" method was used
2000BEC/AUF	"three-step" method was used
2000CER/MIG	Scanning method
2000CER/MIG	Isothermal step method

Correlated heat capacities (42.17.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1968COU/LEE	180.0–355.0	65	0.15		0.860	2.82−2	0.13	1.06−3	−8
1977HOF/SAN	383.1–493.1	12	1.00		0.414	1.42−1	0.41	−4.66−2	−2
1988OKA/OGA	298.1	1	0.40	#	0.171	1.49−2	0.07	1.49−2	1
1997HOV/ROU	298.1	1	0.50	#	0.217	2.36−2	0.11	−2.36−2	−1
2000BEC/AUF	307.0–332.0	6	0.30		0.728	5.46−2	0.22	4.39−2	5
2000BEC/AUF	323.2–363.2	9	0.20		1.642	8.62−2	0.33	−1.70−2	−3
2000CER/MIG	288.1–308.1	4	0.50	#	0.755	7.93−2	0.38	−4.08−2	−2
2000CER/MIG	288.1–308.1	4	0.50	#	0.766	8.04−2	0.38	−4.05−2	−2
2004FEN/PER	298.1	1	1.00		0.536	1.17−1	0.54	1.17−1	1

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1886SCH	(1.94−1, 0.78, 1.72−1, 9)	1898LOU	(4.70−1, 1.76, 4.70−1, 1)
1924WIL/DAN	(6.10−1, 2.20, 5.13−1, 5)	1941ZHD	(4.41−1, 1.88, 3.31−1, 1)
1958SWI/ZIE2	(1.40−1, 0.53, 1.37−1, 2)	1960SWI/ZIE	(2.59−1, 1.07, −2.59−1, −1)
1968PAZ/REC	(8.38−1, 3.43, 6.97−1, 2)	1978RYB/EME	(5.37−1, 2.06, −3.72−1, −3)
1986KOR/KUK	(6.04−2, 0.28, 6.04−2, 1)	1988PIE/SOM1	(1.30−1, 0.60, 1.30−1, 1)
1992NAZ/BAS	(1.67, 6.05, −1.43, −5)		

Parameters of cubic spline polynomials (42.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	140	103	0.922	6.77−2	0.25	−5.80−3	−11
sat	140	103	0.918	6.26−2	0.24	−5.63−3	−12

T/K	A_1	A_2	A_3	A_4	Uncert.
180.0–290.0	7.004 77	1.183 53+1	−6.436 04	1.38412	II
290.0–370.0	1.574 38+2	−1.437 86+2	4.722 63+1	−4.783 98	II
370.0–493.1	−1.886 39+2	1.368 18+2	−2.861 24+1	2.048 34	V
180.0–290.0	7.039 92	1.179 18+1	−6.418 45	1.381 79	II
290.0–370.0	1.578 72+2	−1.442 41+2	4.738 60+1	−4.802 62	II
370.0–493.1	−1.678 97+2	1.198 96+2	−2.400 24+1	1.628 77	V

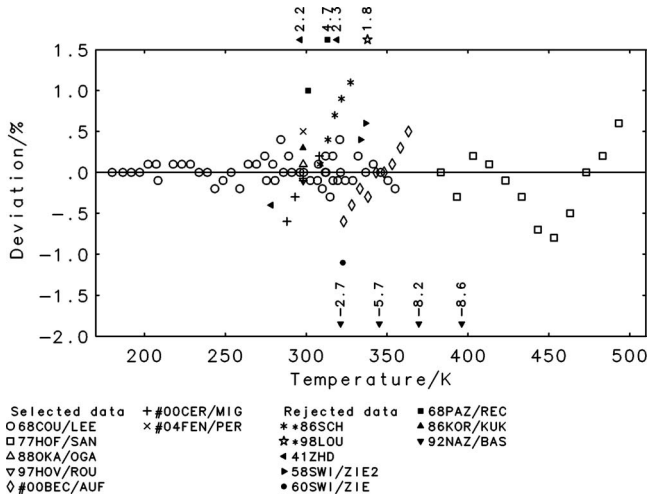

FIG. 84. Deviation plot for 2-methyl-1-propanol (42-017).

Parameters of quasi-polynomial equation (42.17.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	140	103	3.600	4.39−1	1.30	−6.27−3	14

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
180.0–493.1	547.78	3.366 62+2	2.378 03+1	−1.189 63+1	3.594 53+2	−7.103 09+1	4.432 70+2	V

Deviation plot for 2–Methyl—1–propanol (42–017) is given in Fig. 84.

6.5.2.10. 2-Methyl-2-propanol (42-018)

Name:	2-Methyl-2-propanol
Formula:	$C_4H_{10}O$
CAS-RN:	75-65-0
Group No:	42-018

Experimental heat capacities (42.18.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1926PAR/AND		300.0–300.3	2		n/a	n/a	n/a	p	BSIO	1925PAR
1959KEN/TOM		304.6–324.6	2		n/a	n/a	n/a	p	BSIO	1957KEN
1961ROU		304.3–316.7	6		n/a	n/a	n/a	p	BSAO	1961ROU
1963OET		303.6-331.3	12		0.30	99.91	melpt	p	BSAO	1958HIL/KRA
1971REC/SAD		303.1	1		n/a	n/a	n/a	p	BSIO	1970REC
1976SKO/SUU		298.1	1		0.10	n/a	n/a	p	DDCT	1971KON/SUU
1977DEV/PER1		298.1–328.1	3		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1977DEV/PER2		298.1	1		n/a	n/a	n/a	p	FSIT	1971PIC/LED
1977HOF/SAN	N	353.1–453.1	11	S	1.00	n/a	n/a	p	FSIO	1975SAN
1977MUR/SUB		298.1	1		0.30	n/a	n/a	p	BSIO	1964MOE/THO
1988CAC/COS		298.1	1		−1.0	n/a	n/a	p	FSIT	1971PIC/LED
1988OKA/OGA	N	298.1	1		n/a	n/a	n/a	p	FSIO	1985OGA
2003YAN/MA2		298.1–343.1	10		2.00	n/a	n/a	p	BDHT	2004YAN/MA

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference

Reference	Notes
1977HOF/SAN	C_p at saturation curve extrapolated from high pressure measurements
1988OKA/OGA	water content below 0.083 mol %

Correlated heat capacities (42.18.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1963OET	303.6–331.3	12	0.30		0.316	2.68−2	0.09	−2.87−3	−3
1976SKO/SUU	298.1	1	0.10		0.015	4.03−4	0.00	4.03−4	0
1977HOF/SAN	353.1–453.1	11	1.00		0.236	7.65−2	0.24	9.56−3	2
1988CAC/COS	298.1	1	2.00	#	0.749	3.88−1	1.50	−3.88−1	−1
2003YAN/MA2	298.1–343.1	10	2.00		0.257	1.50−1	0.51	1.40−1	10

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1926PAR/AND	(5.14−1, 1.90, 5.13−1, 2)	1959KEN/TOM	(1.13, 4.23, −1.12, −2)
1961ROU	(2.16−1, 0.78, 1.79−1, 4)	1971REC/SAD	(1.76−1, 0.65, 1.76−1, 1)
1977DEV/PER1	(6.11−1, 2.41, −3.45−1, −1)	1977DEV/PER2	(1.03, 4.09, −1.03, −1)
1977MUR/SUB	(7.58−1, 2.80, 7.58−1, 1)	1988OKA/OGA	(3.95−1, 1.48, 3.95−1, 1)

Parameters of cubic spline polynomials (42.18.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	52	35	0.318	1.22−1	0.43	3.11−2	8
sat	52	35	0.325	1.23−1	0.43	2.96−2	6

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–310.0	−2.667 83+3	2.568 98+3	−8.192 42+2	8.743 10+1	II
310.0–453.1	−1.269 98+2	1.101 11+2	−2.605 90+1	2.142 47	III
298.1–310.0	−2.935 44+3	2.829 37+3	−9.036 62+2	9.655 07+1	II
310.0–453.1	−1.068 89+2	9.205 35+1	−2.065 75+1	1.604 00	III

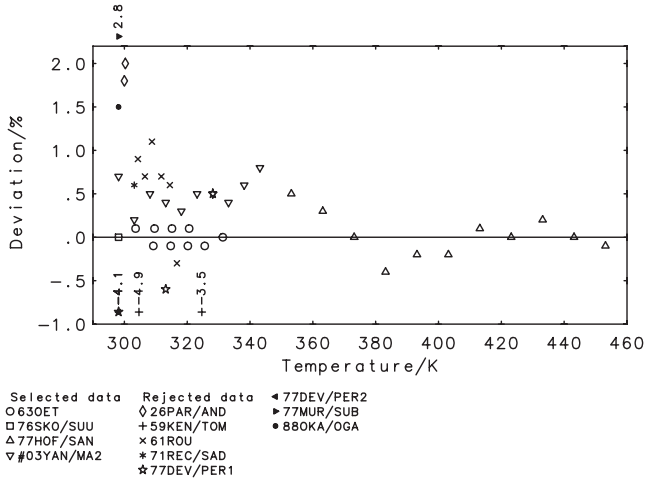

FIG. 85. Deviation plot for 2-methyl-2-propanol (42-018).

Parameters of quasipolynomial equation (42.18.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	52	35	0.738	1.44−1	0.48	−7.83−3	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
298.1–453.1	506.21	3.161 64+1	2.264 38	−1.773 98+2	7.926 20+2	−9.568 09+2	4.471 98+2	IV

Deviation plot for 2–Methyl–2–Propanol (42–018) is given in Fig. 85.

6.5.2.11. 1,3-Butanediol (42-019)

Name:	1,3-Butanediol
Formula:	$C_4H_{10}O_2$
CAS-RN:	107-88-0
Group No:	42-019

Experimental heat capacities (42.19.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1972KAW/OTA		303.1	1		n/a	n/a	n/a	p	BSIO	1949WEI
1996STE/CHI1		300.0–670.0	20	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
1998HAW/GRA		298.1	1		n/a	99.0	chrom	p	BSIO	1998HAW/GRA
2005ZOR/CHO		285.1–353.1	28		n/a	99.0	chrom	p	BDCT	2000ERN/CHO

Correlated heat capacities (42.19.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1996STE/CHI1	300.0–670.0	20	1.00		1.419	6.41−1	1.42	−6.88−2	−6
1998HAW/GRA	298.1	1	1.50	#	0.020	7.81−3	0.03	−7.81−3	−1
2005ZOR/CHO	285.1–353.1	28	1.50	#	0.368	1.53−1	0.55	1.51−1	28

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1972KAW/OTA	(6.98−1, 2.55, 6.98−1, 1)

Parameters of cubic spline polynomials (42.19.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	50	49	1.012	4.54−1	1.07	5.83−2	21
sat	50	49	0.815	2.90−1	0.88	5.22−2	23

T/K	A_1	A_2	A_3	A_4	Uncert.
285.1–450.0	2.262 63+1	−1.11 647+1	6.124 12	−6.603 94−1	III
450.0–635.0	−1.725 44+2	1.189 49+2	−2.279 00+1	1.481 39	III
635.0–670.0	−1.791 86+5	8.469 21+4	−1.334 14+4	7.006 21+2	V
285.1–450.0	2.110 71+1	−9.902 06	5.780 33	−6.298 11−1	IV
450.0–635.0	−1.474 10+2	1.024 42+2	−1.918 51+1	1.219 48	IV
635.0–670.0	−1.054 94+5	4.987 24+4	−7.856 98+3	4.126 52+2	V

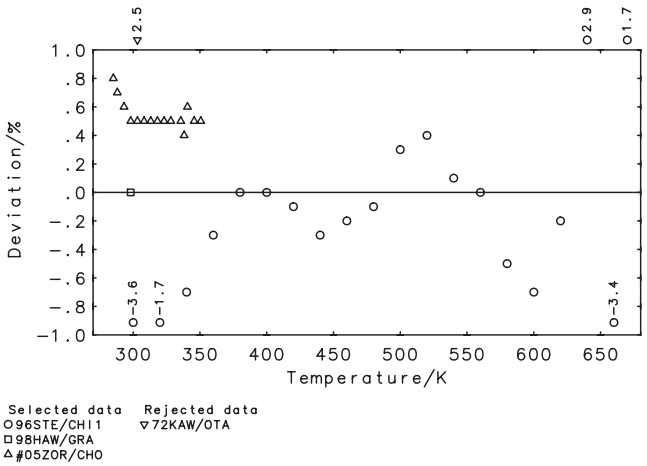

FIG. 86. Deviation plot for 1,3-butanediol (42-019).

Parameters of quasipolynomial equation (42.19.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	50	49	1.096	4.05−1	1.11	−1.50−2	−4

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
285.1–670.0	676.00	1.251 61	3.753 56−1	−2.141 58+1	1.703 03+2	−1.665 23+2	6.007 86+1	IV

Deviation plot for 1,3–Butanediol (42–019) is given in Fig. 86.

6.5.2.12. 1,4-Butanediol (42-020)

Name:	1,4-Butanediol
Formula:	$C_4H_{10}O_2$
CAS-RN:	110-63-4
Group No:	42-020

Experimental heat capacities (42.20.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1974PET/TER		297.8–431.9	14	1.00	98.	melpt	*p*	BDCT	1974PET/TER
1976NIC/SKO		298.1	1	0.20	n/a	n/a	*p*	DDCT	1971KON/SUU
1979NIS/BAB		295.7–315.8	16	0.30	99.48	melpt	*p*	BSAO	1976LEB/LIT
1979NIS/BAB		310.0–450.0	15	0.80	99.48	melpt	*p*	BSAO	1976LEB/LIT
1998HAW/GRA		298.1	1	n/a	99.0	chrom	*p*	BSIO	1998HAW/GRA
2003YAN/MA2		293.1–363.1	15	2.00	n/a	n/a	*p*	BDHT	2004YAN/MA
2004YAN/MA		293.1–353.1	8	1.00	99.5	anal	*p*	BDHT	2004YAN/MA

6.5.2.13. 2,3-Butanediol (42-021)

Name:	2,3-Butanediol
Formula:	$C_4H_{10}O_2$
CAS-RN:	513-85-9
Group No:	42-021

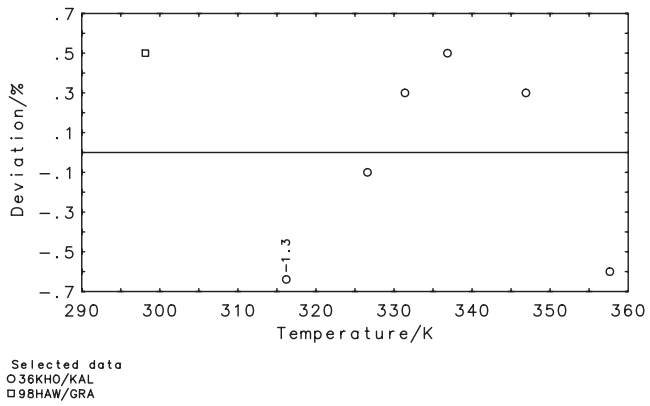

FIG. 87. Deviation plot for 2,3-butanediol (42-021).

Experimental heat capacities (42.21.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KHO/KAL	N	316.2–357.6	7	n/a	n/a	n/a	avg	DSIO	1936KHO/KAL
1998HAW/GRA		298.1	1	n/a	99.0	chrom	p	BSIO	1998HAW/GRA

Reference	Notes
1936KHO/KAL	maximum water content is 0.1%

Correlated heat capacities (42.21.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936KHO/KAL	316.2–357.6	7	1.50	#	0.408	1.73−1	0.61	−1.71−2	1
1998HAW/GRA	298.1	1	1.50	#	0.331	1.35−1	0.50	1.35−1	1

Parameters of regression polynomial (42.21.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	8	8	0.505	2.13−1	0.76	1.90−3	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.1–357.6		1.045 35+2		−5.365 99+1		9.277 94		IV

Deviation plot for 2,3–Butanediol (42–021) is given in Fig. 87.

6.5.2.14. 2-Methyl-1-butanol (42-025)

Name:	2-Methyl-1-butanol
Formula:	$C_5H_{12}O$
CAS-RN:	137-32-6
Group No:	42-025

Experimental heat capacities (42.25.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	347.1	1	n/a	n/a	n/a	avg	DSIO	1898LOU
1949LEE		313.0–343.0	eqn	n/a	n/a	n/a	p	BDHO	1933FER/MIL
1994SVO/CEJ		303.0–326.2	6	0.50	99.8	chrom	p	BSAO	1991SVO/ZAB1
2003CEN/RUZ	N	307.8–337.6	12	1.00	99.92	chrom	p	BDCT	1991BAN/GAR

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FEN/PER		298.1	1	1.00	99.0	anal	p	FSIT	1971PIC/LED
2007STR/VAN		124.1–300.7	199	0.20	99.97	chrom	p	BSAO	1998VAN/VAN

Reference	Notes
1898LOU	average value in the temperature range 295–400 K
2003CEN/RUZ	same data in 1997CEN/RUZ

Correlated heat capacities (42.25.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1898LOU	347.1	1	2.00	#	2.255	1.42	4.51	−1.42	−1
1994SVO/CEJ	303.0–326.2	6	0.50		1.804	2.53−1	0.90	1.55−1	4
2003CEN/RUZ	307.8–337.6	12	1.00		1.074	3.05−1	1.07	1.36−1	6
2004FEN/PER	298.1	1	1.00		1.389	3.59−1	1.39	3.59−1	1
2007STR/VAN	124.1–300.7	199	0.20		0.910	3.59−2	0.18	−8.71−4	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1949LEE	(2.08, 7.24, −1.64, −3)

Parameters of regression polynomial (42.25.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	222	219	0.976	1.35−1	0.47	6.05−3	10	
T/K		A_1		A_2		A_3	A_4	Uncert.
124.1–347.1		1.426 12+1		6.183 33		−4.351 72	1.188 00	IV

Deviation plot for 2–Methyl–1–butanol (42–025) is given in Fig. 88.

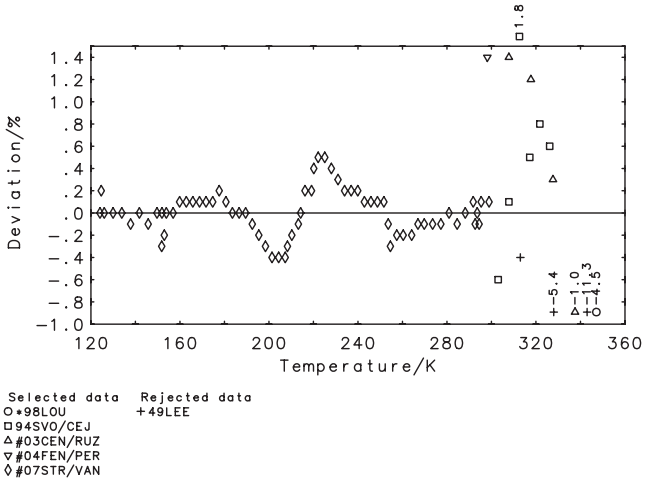

FIG. 88. Deviation plot for 2-methyl-1-butanol (42-025).

6.5.2.15. 2-Methyl-2-butanol (42-026)

Name:	2-Methyl-2-butanol
Formula:	$C_5H_{12}O$
CAS-RN:	75-85-4
Group No:	42-026

Experimental heat capacities (42.26.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	332.4	1	n/a	n/a	n/a	avg	DSIO	1898LOU
1933PAR/HUF		275.0–294.4	4	1.00	n/a	n/a	*p*	BSIO	1925PAR
1949LEE		313.0–343.0	eqn	n/a	n/a	n/a	*p*	BDHO	1933FER/MIL
1983DAP/DEL		288.1–298.1	2	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986BEN/DAR2		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1988PIE/SOM1		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1994SVO/CEJ		303.0–326.2	6	0.50	98.8	chrom	*p*	BSAO	1991SVO/ZAB1
1996TAN/TOY2		298.1	1	n/a	99.99	chrom	*p*	FSIT	1971PIC/LED
2003CEN/RUZ	N	307.9–347.5	10	1.00	99.91	chrom	*p*	BDCT	1991BAN/GAR
2004FEN/PER		298.1	1	1.00	99.0	anal	*p*	FSIT	1971PIC/LED
2007STR/VAN		267.6–300.7	18	0.20	99.99	chrom	*p*	BSAO	1998VAN/VAN

Reference	Notes
1898LOU	average value in the temperature range 293−372 K
2003CEN/RUZ	same data in 1997CEN/RUZ

Correlated heat capacities (42.26.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1933PAR/HUF	275.0–294.4	4	1.00		2.778	7.79−1	2.78	7.73−1	4
1983DAP/DEL	288.1–298.1	2	0.30		7.148	6.21−1	2.14	6.13−1	2
1986BEN/DAR2	298.1	1	0.30		7.593	6.82−1	2.28	6.82−1	1
1988PIE/SOM1	298.1	1	0.50	#	3.204	4.76−1	1.60	4.76−1	1
1994SVO/CEJ	303.0–326.2	6	0.50		1.480	2.37−1	0.74	1.03−1	1
1996TAN/TOY2	298.1	1	0.50	#	5.042	7.56−1	2.52	7.56−1	1
2003CEN/RUZ	307.9–347.5	10	1.00		0.906	2.89−1	0.91	1.11−1	0
2004FEN/PER	298.1	1	1.00		3.150	9.51−1	3.15	9.51−1	1
2007STR/VAN	267.6–300.7	18	0.20		2.097	1.21−1	0.42	−7.07−2	−10

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1898LOU	(8.05−1, 2.41, −8.05−1, −1)	1949LEE	(5.20−1, 1.54, −4.13−1, −1)

Parameters of regression polynomial (42.26.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	48	44	2.902	4.12−1	1.40	1.74−1	1

T/K	A_1	A_2	A_3	A_4	Uncert.
267.6–347.5	6.478 95+2	−6.345 17+2	2.117 79+2	−2.299 35+1	IV

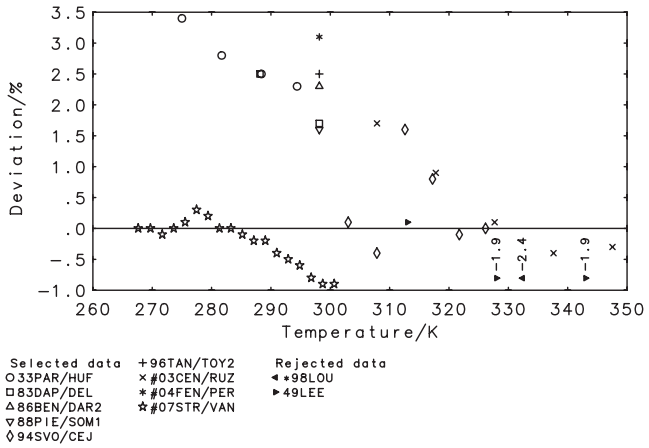

FIG. 89. Deviation plot for 2-methyl-2-butanol (42-026).

Parameters of quasipolynomial equation (42.26.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	48	44	3.866	3.68−1	1.27	3.51−2	−8

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
267.6–347.5	543.70	4.988 04+4	5.268 55+3	−6.924 08+3	5.757 16+4	−1.587 77+4	4.937 16+4	IV

Deviation plot for 2–Methyl–2–butanol (42–026) is given in Fig. 89.

6.5.2.16. 3-Methyl-1-butanol (42-027)

Name:	3-Methyl-1-butanol
Formula:	$C_5H_{12}O$
CAS-RN:	123-51-3
Group No:	42-027

Experimental heat capacities (42.27.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		309.7–337.4	10	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1898LOU	N	348.6	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1907BAT		224.0–263.6	6		n/a	n/a	n/a	p	BSIO	1907BAT
1912LUS	N	321.0	1		n/a	n/a	n/a	avg	DSIO	1912LUS
1924WIL/DAN		303.0–353.0	eqn		n/a	n/a	n/a	p	BSAO	1924WIL/DAN
1945ZHD		280.5–319.9	3		n/a	n/a	n/a	p	BSIT	1934KOL/UDO2
1949LEE		313.0–343.0	eqn		n/a	n/a	n/a	p	BDHO	1933FER/MIL
1958SWI/ZIE2	N	347.5	1		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1990RAO/RAJ		318.1–333.1	4		4.00	n/a	n/a	p	BDHT	1989PRA/RAJ
1992NAZ/BAS		302.0–368.3	4		2.20	98.3	chrom	p	BDHO	1986NAZ/BAS1
1994SVO/CEJ		303.0–326.2	6		0.50	100	chrom	p	BSAO	1991SVO/ZAB1
2003CEN/RUZ	N	307.7–357.4	11		1.00	99.72	chrom	p	BDCT	1991BAN/GAR
2004FEN/PER		298.1	1		1.00	99.0	anal	p	FSIT	1971PIC/LED
2007STR/VAN		138.7–299.4	83		0.20	99.93	chrom	p	BSAO	1998VAN/VAN

Reference	Notes
1898LOU	average value in the temperature range 294–403 K
1912LUS	average value in the temperature range 287–355 K

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1958SWI/ZIE2	average value in the temperature range 295–400 K								
2003CEN/RUZ	same data in 1997CEN/RUZ								

Correlated heat capacities (42.27.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1907BAT	224.0–263.6	6	3.00	#	0.271	1.71−1	0.81	−5.15−3	0
1958SWI/ZIE2	347.5	1	1.00	#	0.262	8.14−2	0.26	−8.14−2	−1
1994SVO/CEJ	303.0–326.2	6	0.50		1.437	1.95−1	0.72	1.30−1	4
2003CEN/RUZ	307.7-357.4	11	1.00		1.037	3.11−1	1.04	2.39−3	3
2004FEN/PER	298.1	1	1.00		1.009	2.54−1	1.01	2.54−1	1
2007STR/VAN	138.7–299.4	83	0.20		0.882	3.50−2	0.18	−1.37−3	6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1886SCH	(4.96−1, 1.76, 4.89−1, 10)	1898LOU	(4.00−1, 1.30, −4.00−1, −1)
1912LUS	(1.98, 6.73, 1.98, 1)	1924WIL/DAN	(5.18−1, 1.73, −4.39−1, −5)
1945ZHD	(3.96−1, 1.55, 3.79−1, 3)	1949LEE	(5.21−1, 1.81, −1.02−1, −1)
1990RAO/RAJ	(1.03, 3.94, −9.00−1, −4)	1992NAZ/BAS	(1.73, 5.76, 1.71, 3)

Parameters of regression polynomial (42.27.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	139	108	0.932	1.26−1	0.47	7.70−3	13	
T/K		A_1		A_2		A_3	A_4	Uncert.
138.7–357.4		1.094 82+1		9.259 29		−4.775 71	1.087 29	IV

Parameters of quasipolynomial equation (42.27.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−					
p	139	60	1.246	8.47−2	0.36	−1.84−2	−7					
T/K		T_c/K		A_1		A_2	A_3	A_4	A_5	A_6	Uncert.	
231.6–357.4		579.40		2.483 92+3		2.367 75+2	−2.541 77+2	2.629 41+3	3.534 27+2	2.401 33+3	IV	

Deviation plot for 3–Methyl—1–butanol (42–027) is given in Fig. 90.

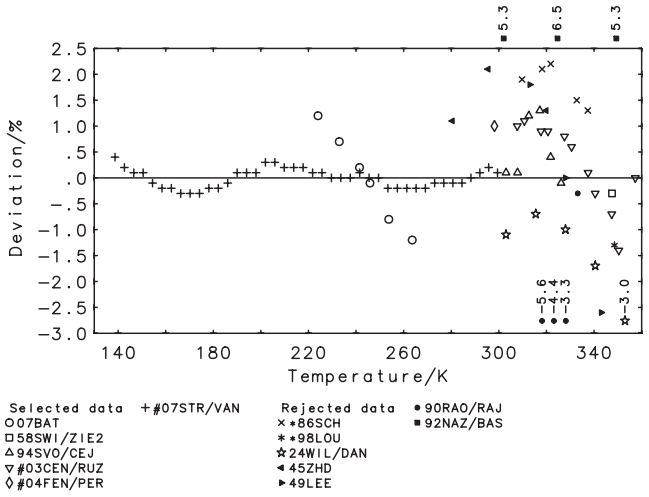

FIG. 90. Deviation plot for 3-methyl-1-butanol (42-027).

6.5.2.17. 3-Methyl-2-butanol (42-028)

Name:	3-Methyl-2-butanol
Formula:	$C_5H_{12}O$
CAS-RN:	598-75-4
Group No:	42-028

Experimental heat capacities (42.28.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991ATR/NES		218.4–370.7	29	n/a	99.9	anal	sat	BSAO	1978ZHU/ATR
1994SVO/CEJ		303.0–326.2	6	0.50	99.6	chrom	*p*	BSAO	1991SVO/ZAB1
2003CEN/RUZ	N	304.2–347.4	16	1.00	99.99	chrom	*p*	BDCT	1991BAN/GAR
2004FEN/PER		298.1	1	1.00	98.0	anal	*p*	FSIT	1971PIC/LED
2007STR/VAN		138.7–300.8	171	0.20	99.93	chrom	*p*	BSAO	1998VAN/VAN

Reference	Notes
2003CEN/RUZ	same data in 1997CEN/RUZ

Correlated heat capacities (42.28.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1991ATR/NES	218.4–370.7	29	1.00	#	0.999	3.35−1	01.00	−4.39−2	−10
2003CEN/RUZ	304.2–347.4	16	1.00		0.622	2.01−1	0.62	−1.67−1	−13
2004FEN/PER	298.1	1	1.00		0.414	1.24−1	0.41	1.24−1	1
2007STR/VAN	138.7–300.8	171	0.20		1.354	5.21−2	0.27	1.14−3	5

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1994SVO/CEJ	(1.01, 3.29, −1.00, −6)

Parameters of cubic spline polynomials (42.28.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	223	217	1.283	1.44−1	0.48	−1.67−2	−17

T/K	A_1	A_2	A_3	A_4	Uncert.
138.7–250.0	6.447 55	1.795 99+1	−1.144 98+1	2.756 89	II
250.0–370.7	2.020 52+2	−2.167 65+2	8.244 01+1	−9.761 77	IV

Parameters of quasi-polynomial equation (42.28.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	223	168	1.246	1.02−1	0.37	5.67−3	9

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
190.3–370.7	556.10	8.131 06+3	9.353 74+2	−9.624 65+2	7.723 83+3	9.528 07+2	5.235 69+3	IV

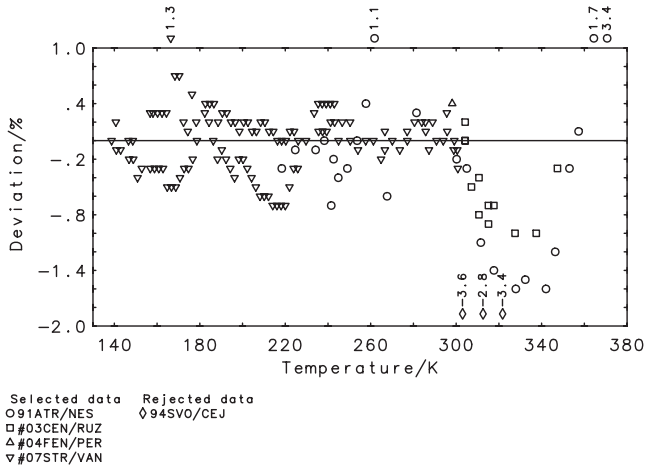

FIG. 91. Deviation plot for 3-methyl-2-butanol (42-028).

Deviation plot for 3–Methyl—2–butanol (42–028) is given in Fig. 91.

6.5.2.18. 1-Pentanol (42-029)

Name:	1-Pentanol
Formula:	$C_5H_{12}O$
CAS-RN:	71-41-0
Group No:	42-029

Experimental heat capacities (42.29.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1933PAR/HUF		204.1–298.0	6		1.00	n/a	n/a	*p*	BSIO	1925PAR
1939PHI	N	302.4	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1949LEE		313.0–343.0	eqn		n/a	n/a	n/a	*p*	BDHO	1933FER/MIL
1949TSC/RIC2		298.1	1		n/a	n/a	n/a	*p*	BSIO	1949TSC/RIC1
1968COU/LEE		205.1–389.1	53		0.15	99.87	melpt	*p*	BSAO	1963AND/COU1
1968PAZ/REC	N	313.1	1		n/a	n/a	n/a	*p*	BDCT	1970PAZ/PAZ
1976SKO/SUU		298.1	1		0.10	n/a	n/a	*p*	DDCT	1971KON/SUU
1979GRI/YAN	N	301.3–463.4	9		0.90	n/a	n/a	*p*	BDAO	1975RAS/GRI
1981ARU/BAG		293.1–393.1	6	S	1.50	n/a	n/a	*p*	BDHT	1981ARU
1983DAP/DEL		288.1–298.1	2		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1983PFE/SCH		298.1	1		n/a	n/a	n/a	*p*	BDCT	1968WAD
1984ZEG/SOM2		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1986BEN/DAR2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1986TAN/TOY		298.1	1		0.30	98.	anal	*p*	FSIT	1971PIC/LED
1999CAL/BRO		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
2004FEN/PER		298.1	1		1.00	99.0	anal	*p*	FSIT	1971PIC/LED
2004VAN/VAN	N	198.6–380.8	184		0.20	99.8	melpt	*p*	BSAO	1987VAN/VAN

Reference	Notes
1939PHI	isomer n/a, 1-alkanol assumed
1968PAZ/REC	same datum in 1970PAZ/PAZ
1979GRI/YAN	data above 382.68 K were measured at elevated pressures up to 0.81 MPa

Correlated heat capacities (42.29.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1968COU/LEE	205.1–389.1	53	0.15		0.527	1.98−2	0.08	−1.07−2	−23
1976SKO/SUU	298.1	1	0.10		0.552	1.38−2	0.06	1.38−2	1
1979GRI/YAN	301.3–463.4	9	0.90		0.676	1.95−1	0.61	1.34−1	5
1986TAN/TOY	298.1	1	0.30		0.152	1.14−2	0.05	−1.14−2	−1
1999CAL/BRO	298.1	1	0.30	#	0.024	1.80−3	0.01	−1.80−3	0
2004FEN/PER	298.1	1	1.00		0.247	6.19−2	0.25	6.19−2	1
2004VAN/VAN	198.6–380.8	184	0.20		0.562	3.04−2	0.11	2.20−3	16

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1933PAR/HUF	(5.98−2, 0.24, 4.95−2, 6)	1939PHI	(1.20, 4.94, −1.20, −1)
1949LEE	(1.54, 5.69, −1.48, −8)	1949TSC/RIC2	(6.77−1, 2.63, 6.77−1, 1)
1968PAZ/REC	(2.33, 8.06, 2.33, 1)	1981ARU/BAG	(4.00−1, 1.39, −3.03−1, −4)
1983DAP/DEL	(9.42−2, 0.38, −8.97−2, −2)	1983PFE/SCH	(7.57−2, 0.30, 7.57−2, 1)
1984ZEG/SOM2	(8.36−2, 0.33, 8.36−2, 1)	1986BEN/DAR2	(1.00−1, 0.40, −1.00−1, −1)

Parameters of cubic spline polynomials (42.29.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	278	250	0.562	4.69−2	0.16	6.45−3	28
sat	278	250	0.565	4.70−2	0.16	6.47−3	25

T/K	A_1	A_2	A_3	A_4	Uncert.
198.7–295.0	1.351 09+1	8.537 94	−5.068 74	1.175 01	II
295.0–380.0	1.598 51+2	−1.402 83+2	4.537 89+1	−4.525 29	II
380.0–463.4	−2.762 98+2	2.040 45+2	−4.523 37+1	3.423 19	IV
198.7–295.0	1.337 07+1	8.707 08	−5.136 01	1.183 83	II
295.0–380.0	1.606 34+2	−1.410 52+2	4.562 98+1	−4.552 41	II
380.0–463.4	−2.709 13+2	1.996 43+2	−4.402 69+1	3.312 20	IV

Parameters of quasipolynomial equation (42.29.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	278	250	1.339	1.01−1	0.31	1.75−3	7

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
198.6–463.4	588.15	9.604 65+2	8.338 70+1	−7.286 26+1	9.881 32+2	−7.595 00+1	9.718 73+2	IV

Deviation plot for 1–Pentanol (42–029) is given in Fig. 92.

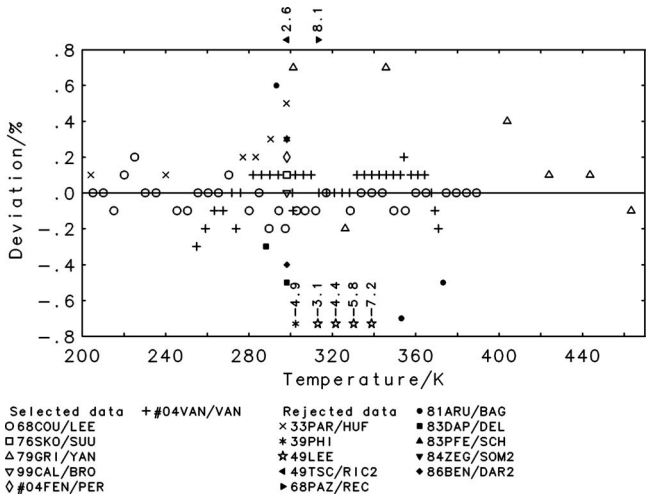

FIG. 92. Deviation plot for 1-pentanol (42-029).

6.5.2.19. 2-Pentanol (42-030)

Name:	2-Pentanol
Formula:	$C_5H_{12}O$
CAS-RN:	6032-29-7
Group No:	42-030

Experimental heat capacities (42.30.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1938PAN/DUD	N	298.0–363.0	eqn	n/a	n/a		p	n/a	
1994SVO/CEJ		303.0–326.2	6	0.50	99.6	chrom	p	BSAO	1991SVO/ZAB1
1996TAN/TOY2		298.1	1	n/a	99.8	chrom	p	FSIT	1971PIC/LED
2003CEN/RUZ	N	307.8–367.4	20	1.00	99.93	chrom	p	BDCT	1991BAN/GAR
2004FEN/PER		298.1	1	1.00	98.0	anal	p	FSIT	1971PIC/LED
2007STR/VAN		137.2–301.1	147	0.20	99.99	chrom	p	BSAO	1998VAN/VAN

Reference	Notes
1938PAN/DUD	temperature range of parameters validity estimated by the compilers
2003CEN/RUZ	same data in 1997CEN/RUZ

Correlated heat capacities (42.30.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1994SVO/CEJ	303.0–326.2	6	0.50		1.358	1.97−1	0.68	−1.07−1	−2
1996TAN/TOY2	298.1	1	0.30	#	1.723	1.46−1	0.52	1.46−1	1
2003CEN/RUZ	307.8–367.4	20	1.00		0.464	1.54−1	0.46	1.21−2	−4
2004FEN/PER	298.1	1	1.00		0.893	2.53−1	0.89	2.53−1	1
2007STR/VAN	137.2–301.1	147	0.20		1.589	6.68−2	0.32	5.49−4	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1938PAN/DUD	(4.25−1, 1.38, 8.85−2, 0)

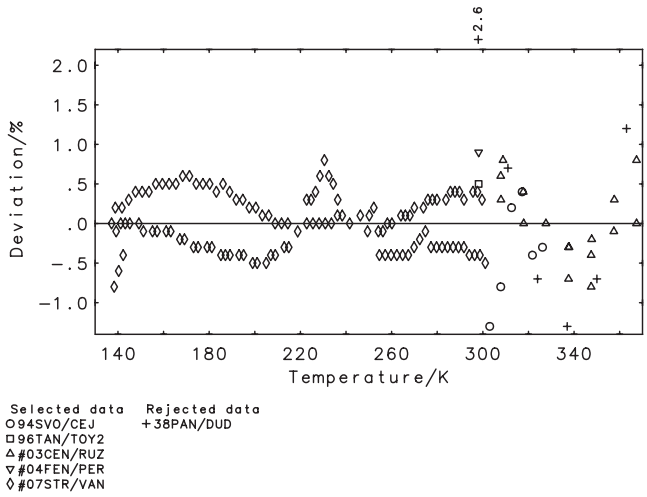

FIG. 93. Deviation plot for 2-pentanol (42-030).

Parameters of cubic spline polynomials (42.30.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	181	175	1.515	9.23−2	0.37	4.36−4	−8

T/K	A_1	A_2	A_3	A_4	Uncert.
137.2–280.0	1.900 93+1	−2.552 73−1	−1.992 99	1.040 67	II
280.0–367.4	2.609 71+2	−2.595 00+2	9.059 43+1	−9.981 64	IV

Deviation plot for 2–Pentanol (42–030) is given in Fig. 93.

6.5.2.20. 3-Pentanol (42-031)

Name:	3-Pentanol
Formula:	$C_5H_{12}O$
CAS-RN:	584-02-1
Group No:	42-031

Experimental heat capacities (42.31.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1949LEE		313.0–343.0	eqn	n/a	n/a		*p*	BDHO	1933FER/MIL
1976CON/GIA		298.1	1	n/a	n/a		*p*	BDCT	1976CON/GIA
1994SVO/CEJ		303.0–326.2	6	0.50	99.6	chrom	*p*	BSAO	1991SVO/ZAB1
1996TAN/TOY2		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
2003CEN/RUZ	N	307.8–367.7	11	1.00	99.90	chrom	*p*	BDCT	1991BAN/GAR
2004FEN/PER		298.1	1	1.00	98.0	anal	*p*	FSIT	1971PIC/LED
2007STR/VAN		210.2–309.3	98	0.20	99.96	chrom	*p*	BSAO	1998VAN/VAN

Reference	Notes
2003CEN/RUZ	same data in 1997CEN/RUZ

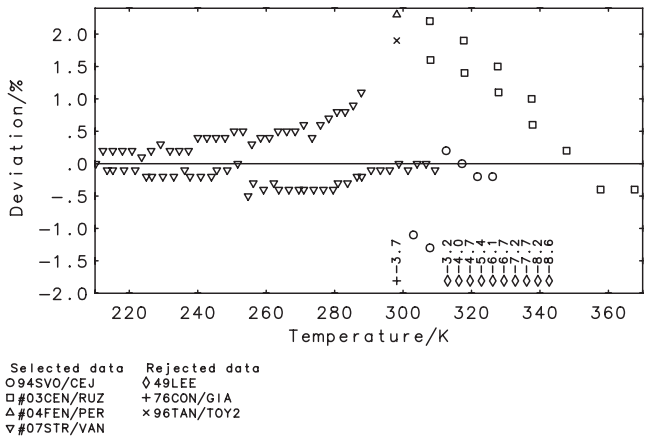

FIG. 94. Deviation plot for 3-pentanol (42-031).

Correlated heat capacities (42.31.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1994SVO/CEJ	303.0–326.2	6	0.50	1.406	2.16−1	0.70	−1.39−1	−4
2003CEN/RUZ	307.8–367.7	11	1.00	1.300	4.28−1	1.30	3.26−1	7
2004FEN/PER	298.1	1	1.00	2.341	7.17−1	2.34	7.17−1	1
2007STR/VAN	210.2–309.4	98	0.20	1.689	8.77−2	0.34	2.87−4	−31

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1949LEE	(2.04, 6.42, −1.96, −10)	1976CON/GIA	(1.07, 3.71, −1.07, −1)
1996TAN/TOY2	(5.71−1, 1.88, 5.71−1, 1)		

Parameters of cubic spline polynomials (42.31.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	128	116	1.694	1.80−1	0.59	3.02−2	−27

T/K	A_1	A_2	A_3	A_4	Uncert.
210.2–260.0	−1.061 51+1	4.159 34+1	−2.171 41+1	4.185 54	II
260.0–280.0	4.712 28+2	−5.143 79+2	1.921 21+2	−2.322 93+1	II
280.0–367.7	1.876 35+1	−2.959 59+1	1.898 46+1	−2.617 75	IV

Deviation plot for 3–Pentanol (42–031) is given in Fig. 94.

6.5.2.21. 1,5-Pentanediol (42-033)

Name:	1,5-Pentanediol
Formula:	$C_5H_{12}O_2$
CAS-RN:	111-29-5
Group No:	42-033

Experimental heat capacities (42.33.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1934MIL	N	269.8–287.0	2	n/a	n/a		avg	BSIO	1920GIB/LAT
1976NIC/SKO		298.1	1	0.20	n/a		p	DDCT	1971KON/SUU

Reference	Notes
1934MIL	average values in the temperature ranges 253–287 and 271–303 K

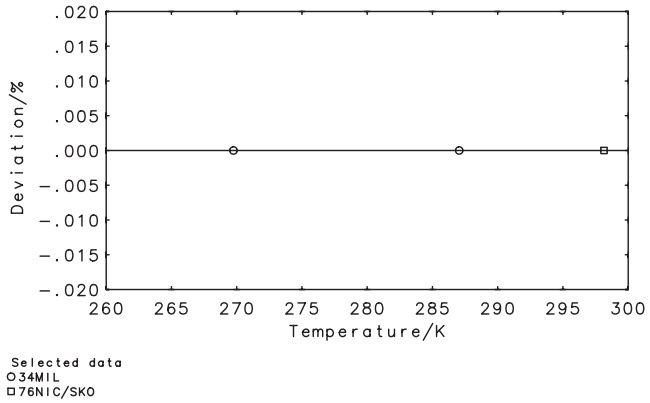

FIG. 95. Deviation plot for 1,5-pentanediol (42-033).

Correlated heat capacities (42.33.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1934MIL	269.8–287.0	2	1.00	#	0.000	4.20−5	0.00	4.20−5	0
1976NIC/SKO	298.1	1	0.20		0.001	5.91−5	0.00	5.91−5	0

Parameters of regression polynomial (42.33.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	3	3	0.000	0.00	0.00	4.77−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
269.8–298.1	4.747 10+2	−3.324 26+2	6.124 93+1		I

Deviation plot for 1,5–Pentanediol (42–033) is given in Fig. 95.

6.5.2.22. 3,3-Dimethyl-1-butanol (42-039)

Name:	3,3-Dimethyl-1-butanol
Formula:	$C_6H_{14}O$
CAS-RN:	624-95-3
Group No:	42-039

Experimental heat capacities (42.39.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1986BEN/KUM		298.1	1	n/a	99.	chrom	p	FSIT	1971PIC/LED
2004MAS/NAK		239.2–301.6	27	0.25	n/a		p	BSAO	1992SOR/KAJ

Correlated heat capacities (42.39.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1986BEN/KUM	298.1	1	0.30	#	4.179	3.56−1	1.25	−3.56−1	−1
2004MAS/NAK	239.2–301.6	27	0.25		0.497	3.51−2	0.12	9.47−3	3

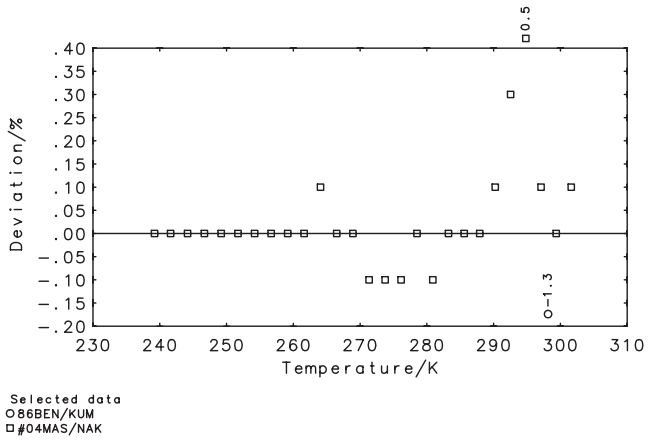

FIG. 96. Deviation plot for 3,3-dimethyl-1-butanol (42-039).

Parameters of regression polynomial (42.39.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−	
p	28	28	0.982	8.00−2	0.28	−3.58−3	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
239.2–301.6		4.046 25+1		−1.951 86+1		5.228 95		IV

Deviation plot for 3,3–Dimethyl–1–butanol (42–039) is given in Fig. 96.

6.5.2.23. 1-Hexanol (42-041)

Name:	1-Hexanol
Formula:	$C_6H_{14}O$
CAS-RN:	111-27-3
Group No:	42-041

Experimental heat capacities (42.41.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1929KEL2		229.6–290.0	7		1.00	n/a		p	BSIO	1929KEL1
1959HUT/BAI		298.1	1		n/a	n/a		p	BSIO	1955HUT/MAN
1973KAL/WOY		303.1	1		n/a	n/a		p	BSIO	1970REC
1979GRI/YAN	N	303.7–462.0	9		0.90	n/a		p	BDAO	1975RAS/GRI
1981ARU		293.1–393.1	6	S	1.50	n/a		p	BDHT	1981ARU
1983BEN/DAR		298.1	1		0.30	n/a		p	FSIT	1971PIC/LED
1984BRA/PIN		298.1	1		n/a	99.	melpt	p	FSIT	1971PIC/LED
1984KAL/WOY		229.1–300.6	35		n/a	99.9	chrom	p	BSAO	1980KAL/JED
1984ZEG/SOM2		298.1	1		n/a	99.	chrom	p	FSIT	1971PIC/LED
1985COS/PAT8		283.1–313.1	3		0.30	98.	estim	p	FSIT	1971PIC/LED\
1986ORT		298.1	1		1.00	99.	anal	p	BDCT	1970PAZ/PAZ
1986TAN/TOY		298.1	1		0.30	98.	anal	p	FSIT	1971PIC/LED
1988AND/PAT		298.1	1		n/a	98.	anal	p	FSIT	1971PIC/LED
1989VES/BAR	N	298.1–318.1	5		0.50	n/a		p	BSAO	1979VES/ZAB
1991ATR/NES		227.3–362.6	20		n/a	99.9	anal	sat	BSAO	1978ZHU/ATR
1998RUZ/MAJ		304.2–349.9	25		1.00	99.60	chrom	p	BDCT	1991BAN/GAR
1999CAL/BRO		298.1	1		n/a	99.0	chrom	p	FSIT	1971PIC/LED
2003VAN/GAB		228.8–399.3	89		0.20	99.8	melpt	p	BSAO	1998VAN/VAN

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference

Reference	Notes
1979GRI/YAN	data above 385.43 K measured at elevated pressures up to 0.74 MPa
1989VES/BAR	water content is 0.04 mass %

6.5.2.24. 3-Methyl-3-pentanol (42-047)

Name:	3-Methyl-3-pentanol
Formula:	$C_6H_{14}O$
CAS-RN:	77-74-7
Group No:	42-047

Experimental heat capacities (42.47.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1979MAR/BRA		298.1	1	1.00	n/a		*p*	BDCT	1970PAZ/PAZ
1984BRA/PIN		298.1	1	0.30	n/a		*p*	FSIT	1971PIC/LED
1986ORT		298.1	1	1.00	98.	anal	*p*	BDCT	1970PAZ/PAZ
1988CAC/COS		283.1–323.1	4	n/a	n/a		*p*	FSIT	1971PIC/LED
2002CER/TOV		278.1–335.6	24	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2004CER/GON	N	278.1–368.1	19	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2004CER/GON	N	288.1–373.1	18	n/a	99.0	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
2004CER/GON	data in supporting information

Correlated heat capacities (42.47.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979MAR/BRA	298.1	1	1.00		0.667	2.40−1	0.67	2.40−1	1
1986ORT	298.1	1	1.00		1.243	4.39−1	1.24	−4.39−1	−1
2002CER/TOV	278.1–335.6	24	1.00	#	0.115	4.09−2	0.11	−6.05−3	−5
2004CER/GON	278.1–368.1	19	1.00	#	0.497	1.96−1	0.50	−1.35−1	−15
2004CER/GON	288.1–373.1	18	1.00	#	0.551	2.17−1	0.55	1.67−1	12

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1984BRA/PIN	(4.93−1, 1.40, −4.93−1, −1)	1988CAC/COS	(7.44−1, 1.92, 6.84−1, 4)

Parameters of regression polynomial (42.47.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	68	63	0.460	1.78−1	0.46	1.59−3	−8		
T/K		A_1		A_2		A_3		A_4	Uncert.
278.1–373.1	−1.771 74+2	1.359 46+2		−2.474 16+1		1.040 13		III	

Deviation plot for 3–Methyl-3–pentanol (42–047) is given in Fig. 97.

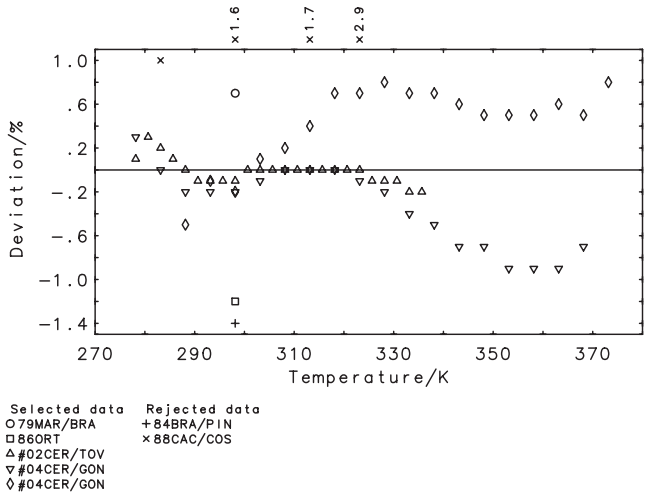

FIG. 97. Deviation plot for 3-methyl-3-pentanol (42-047).

6.5.2.25. Benzenemethanol (42-051)

Name:	Benzenemethanol
Formula:	C_7H_8O
CAS-RN:	100-51-6
Group No:	42-051

Experimental heat capacities (42.51.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		323.0–391.7	5	S	n/a	n/a		avg	DSIO	1881VON
1898LOU	N	384.1	1		n/a	n/a		avg	DSIO	1898LOU
1902LOU1	N	380.6	1		n/a	n/a		avg	DSIO	1898LOU
1931SMI/AND1		259.8–298.5	4		n/a	99.	estim	*p*	DSIO	1926AND/LYN
1936PAR/TOD1		260.0–300.0	5	S	0.70	n/a		*p*	BSIO	1925PAR
1947SKU		293.1	1		0.30	n/a		*p*	BSAO	1947SKU
1975NIC/WAD		298.1	1		n/a	99.5	chrom	*p*	BSIO	1970LKB/COM
1979GRI/YAN		307.5–461.7	9		0.90	n/a		*p*	BDAO	1975RAS/GRI
1986KRU/FED		373.1	1		n/a	n/a		*p*	BDHT	1968OST/DOB
2005FRA/BIG		298.1–318.1	3		n/a	99.8	chrom	*p*	BDHT	1995DIO/MAN

Reference	Notes
1898LOU	average value in the temperature range 295–473 K
1902LOU1	average value in the temperature range 293–468 K

6.5.2.26. 3-Ethyl-3-pentanol (42-062)

Name:	3-Ethyl-3-pentanol
Formula:	$C_7H_{16}O$
CAS-RN:	597-49-9
Group No:	42-062

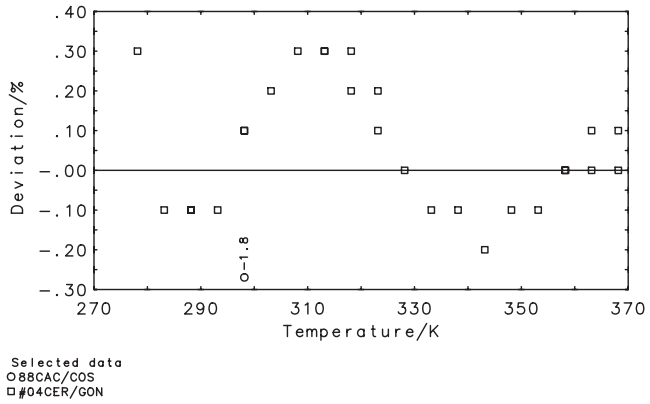

FIG. 98. Deviation plot for 3-ethyl-3-pentanol (42-062).

Experimental heat capacities (42.62.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1988CAC/COS		298.1	1	n/a	n/a		*p*	FSIT	1971PIC/LED
2004CER/GON	N	278.1–368.1	38	n/a	98.0	anal	*p*	BDHT	1969PER/COM

Reference	Notes
2004CER/GON	data in supporting information

Correlated heat capacities (42.62.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1988CAC/COS	298.1	1	1.00	#	1.793	7.63−1	1.79	−7.63−1	−1
2004CER/GON	278.1–368.1	38	1.00	#	0.156	6.79−2	0.16	2.10−2	4

Parameters of regression polynomial (42.62.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	39	39	0.344	1.47−1	0.34	8.67−4	3		
T/K		A_1		A_2		A_3		A_4	Uncert.
278.1–368.1		−7.716 52+2		6.968 22+2		−1.967 37+2		1.834 72+1	III

Deviation plot for 3–Ethyl–3–pentanol (42–062) is given in Fig. 98.

6.5.2.27. 1-Heptanol (42-063)

Name:	1-Heptanol
Formula:	$C_7H_{16}O$
CAS-RN:	111-70-6
Group No:	42-063

Experimental heat capacities (42.63.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1956PAR/KEN		240.0–300.0	7	S	1.00	98.2	melpt	*p*	BSIO	1925PAR
1959HUT/BAI		298.1	1		n/a	n/a		*p*	BSIO	1955HUT/MAN
1967GRA		308.1–338.1	4		1.00	n/a		*p*	BSIO	1967GRA
1979GRI/YAN	N	303.0–462.3	9		0.90	n/a		*p*	BDAO	1975RAS/GRI

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1980VAS/TRE		323.0–453.0	eqn	2.00	99.8	anal	sat	BSAO	1980VAS/TRE
1984ZEG/SOM2		298.1	1	n/a	99.5	chrom	p	FSIT	1971PIC/LED
1988AND/PAT		298.1	1	n/a	98.	anal	p	FSIT	1971PIC/LED
1988ARU/MOV		293.1–433.1	8	3.00	n/a		p	BDHT	1981ARU
1988NAZ/BAS		303.4–447.1	7	2.20	99.2	anal	p	BDHO	1986NAZ/BAS1
1989VES/BAR	N	298.1–318.1	5	0.50	n/a		p	BSAO	1979VES/ZAB
1998RUZ/MAJ		304.3–406.0	34	1.00	99.34	chrom	p	BDCT	1991BAN/GAR
1999CAL/BRO		298.1	1	n/a	99.0	chrom	p	FSIT	1971PIC/LED
2000FUL/RUZ		330.6–570.7	13	2.00	99.94	chrom	sat	BDCT	1991BAN/GAR
2003VAN/GAB	N	241.6–369.7	78	0.20	99.78	melpt	p	BSAO	1998VAN/VAN

Reference	Notes
1979GRI/YAN	data above 425.19 K were measured at elevated pressures up to 0.27 MPa
1989VES/BAR	water content is 0.007 mass %

Correlated heat capacities (42.63.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1956PAR/KEN	240.0–300.0	7	1.00		0.836	2.73−1	0.84	2.24−1	7
1959HUT/BAI	298.1	1	1.00	#	0.348	1.14−1	0.35	−1.14−1	−1
1979GRI/YAN	303.0–462.3	9	1.50	#	0.823	5.49−1	1.24	4.66−1	9
1984ZEG/SOM2	298.1	1	0.50	#	0.363	5.97−2	0.18	−5.97−2	−1
1988AND/PAT	298.1	1	1.50	#	0.459	2.26−1	0.69	−2.26−1	−1
1989VES/BAR	298.1–318.1	5	0.50		2.091	3.52−1	1.05	−3.51−1	−5
1998RUZ/MAJ	304.3–406.0	34	1.00		0.249	1.01−1	0.25	−2.96−2	−6
1999CAL/BRO	298.1	1	0.50	#	1.201	1.97−1	0.60	−1.97−1	−1
2000FUL/RUZ	330.6–570.7	13	2.00		0.120	1.09−1	0.24	−7.90−2	−8
2003VAN/GAB	241.6–369.7	78	0.20		0.677	4.94−2	0.14	3.38−3	22

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1967GRA	(9.31−1, 2.71, −8.91−1, −4)	1980VAS/TRE	(6.61−1, 1.69, −5.11−1, −9)
1988ARU/MOV	(1.99, 4.03, 8.40−1, −2)	1988NAZ/BAS	(1.29, 3.32, 4.88−1, 1)

Parameters of cubic spline polynomials (42.63.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	182	150	0.711	1.80−1	0.45	1.10−2	15
sat	182	150	0.712	1.80−1	0.45	1.03−2	17

T/K	A_1	A_2	A_3	A_4	Uncert.
240.0–320.0	8.826 73+1	−6.580 74+1	2.168 00+1	−1.954 80	II
320.0–380.0	2.477 28+2	−2.153 02+2	6.839 72+1	−6.821 17	II
380.0–570.7	−3.063 13+2	2.220 99+2	−4.670 84+1	3.275 81	IV
240.0–320.0	8.857 01+1	−6.612 76+1	2.179 23+1	−1.967 83	II
320.0–380.0	2.463 69+2	−2.140 64+2	6.802 25+1	−6.783 48	II
380.0–570.7	−2.958 45+2	2.140 00+2	−4.462 59+1	3.097 96	IV

Deviation plot for 1–Heptanol (42–063) is given in Fig. 99.

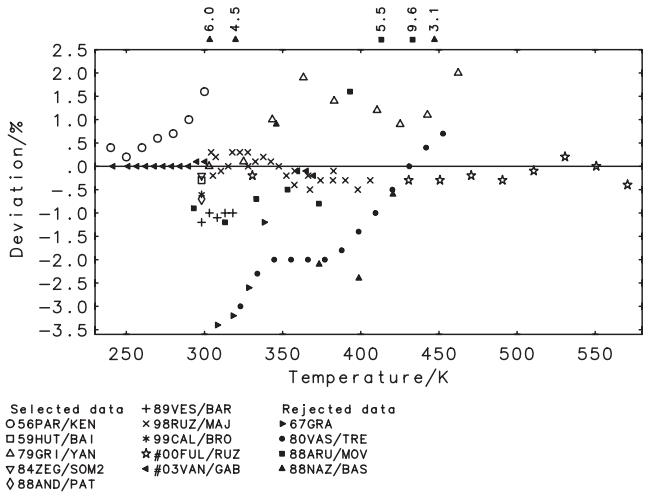

FIG. 99. Deviation plot for 1-heptanol (42-063).

6.5.2.28. Benzeneethanol (42-066)

Name:	Benzeneethanol
Formula:	$C_8H_{10}O$
CAS-RN:	60-12-8
Group No:	42-066

Experimental heat capacities (42.66.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1975NIC/WAD		298.1	1	n/a	99.5	chrom	*p*	BSIO	1970LKB/COM
2005FRA/BIG		298.1–318.1	3	n/a	99.0	error	*p*	BDHT	1995DIO/MAN

6.5.2.29. 1-Octanol (42-079)

Name:	1-Octanol
Formula:	$C_8H_{18}O$
CAS-RN:	111-87-5
Group No:	42-079

Experimental heat capacities (42.79.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		314.2–384.8	5	S	n/a	n/a		avg	DSIO	1881VON
1931CLI/AND		246.0–286.0	4		n/a	n/a		sat	DSIO	1926AND/LYN
1959HUT/BAI		298.1	1		n/a	n/a		*p*	BSIO	1955HUT/MAN
1961ROU		298.9–311.3	5		n/a	n/a		*p*	BSAO	1961ROU
1979GRI/YAN		310.7–452.3	8		0.90	n/a		*p*	BDAO	1975RAS/GRI
1980VAS/TRE		313.0–468.0	eqn		2.00	99.6	anal	sat	BSAO	1980VAS/TRE
1983PFE/SCH		298.1	1		n/a	n/a		*p*	BDCT	1968WAD
1984ZEG/SOM2		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1986NAZ/BAS2		303.2–448.6	7		2.00	99.6	estim	*p*	BDHO	1986NAZ/BAS1
1989VES/BAR	N	298.1–318.1	5		0.50	n/a		*p*	BSAO	1979VES/ZAB
1992PFE/SCH		298.1–313.1	2		n/a	n/a		*p*	BDCT	1968WAD
1998RUZ/MAJ		304.3–367.4	32		1.00	99.90	chrom	*p*	BDCT	1991BAN/GAR
1999CAL/BRO		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED
2000FUL/RUZ		330.6–550.7	12		2.00	99.94	chrom	sat	BDCT	1991BAN/GAR

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003VAN/GAB		260.7–397.5	67	0.20	99.82	melpt	p	BSAO	1998VAN/VAN

Reference	Notes
1989VES/BAR	water content is 0.039 mass %

Correlated heat capacities (42.79.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979GRI/YAN	310.7–452.3	8	0.90		0.772	3.12−1	0.69	1.83−2	−2
1998RUZ/MAJ	304.3–367.4	32	1.00		0.649	2.67−1	0.65	−2.63−1	−32
1999CAL/BRO	298.1	1	0.50	#	1.736	3.19−1	0.87	−3.19−1	−1
2000FUL/RUZ	330.6–550.7	12	2.00		0.183	1.78−1	0.37	−6.94−2	−3
2003VAN/GAB	260.7–397.5	67	0.20		0.311	2.41−2	0.06	5.96−3	4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1881VON	(2.85, 6.45, −2.30, −3)	1931CLI/AND	(1.07, 3.14, −1.00, −2)
1959HUT/BAI	(6.09−1, 1.62, 6.09−1, 1)	1961ROU	(2.53−1, 0.67, −2.21−1, −5)
1980VAS/TRE	(6.50−1, 1.48, −5.79−1, −12)	1983PFE/SCH	(2.57, 7.47, −2.57, −1)
1984ZEG/SOM2	(2.83−1, 0.77, −2.83−1, −1)	1986NAZ/BAS2	(1.30, 2.93, 4.37−2, −1)
1989VES/BAR	(5.18−1, 1.37, −5.17−1, −5)	1992PFE/SCH	(4.91−1, 1.35, −3.27−1, 0)

Parameters of cubic spline polynomials (42.79.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	164	120	0.495	1.77−1	0.42	−7.51−2	−34
sat	164	120	0.495	1.77−1	0.42	−7.52−2	−33

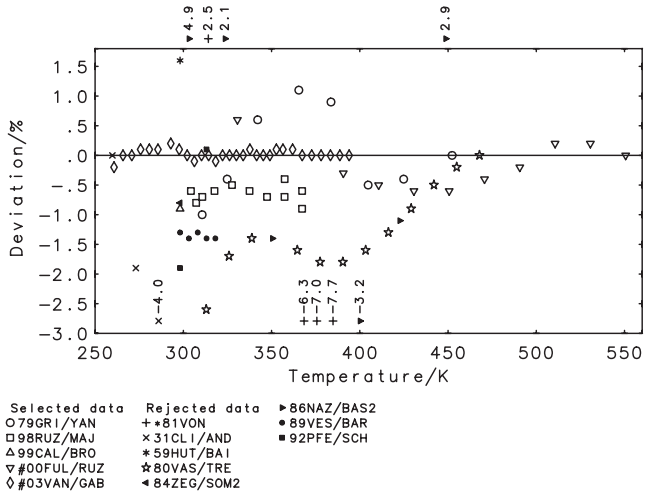

FIG. 100. Deviation plot for 1-octanol (42-079).

T/K	A_1	A_2	A_3	A_4	Uncert.
260.7–390.0	1.798 04+2	−1.541 31+2	5.102 85+1	−5.163 15	II
390.0–550.6	−3.246 99+2	2.339 49+2	−4.847 91+1	3.341 78	IV
260.7–390.0	1.798 33+2	−1.541 58+2	5.103 70+1	−5.164 02	II
390.0–550.6	−3.200 88+2	2.303 97+2	−4.756 68+1	3.263 65	IV

Deviation plot for 1–Octanol (42–079) is given in Fig. 100.

6.5.2.30. Benzenepropanol (42-083)

Name:	Benzenepropanol
Formula:	$C_9H_{12}O$
CAS-RN:	122-97-4
Group No:	42-083

Experimental heat capacities (42.83.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1975NIC/WAD		298.1	1	n/a	99.5	chrom	*p*	BSIO	1970LKB/COM
2005FRA/BIG		298.1–318.1	3	n/a	99.0	error	*p*	BDHT	1995DIO/MAN

6.5.2.31. 1-Nonanol (42-084)

Name:	1-Nonanol
Formula:	$C_9H_{20}O$
CAS-RN:	143-08-8
Group No:	42-084

Experimental heat capacities (42.84.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1979GRI/YAN		304.2–464.2	10	0.90	n/a		*p*	BDAO	1975RAS/GRI
1982VAS/PET		303.0–423.0	eqn	n/a	99.2	anal	sat	BSAO	1980VAS/TRE
1982VAS/PET		423.0–483.0	eqn	n/a	99.2	anal	sat	BSAO	1980VAS/TRE
1986NAZ/BAS2		303.1–474.1	8	2.00	99.4	estim	*p*	BDHO	1986NAZ/BAS1
1999CAL/BRO		298.1	1	n/a	98.0	anal	*p*	FSIT	1971PIC/LED
2005DOM/MAR		281.1–330.1	24	n/a	98.	chrom	*p*	BDCT	1989BRE/LIC

Correlated heat capacities (42.84.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979GRI/YAN	325.2–464.2	8	0.90		0.498	2.15−1	0.45	2.44−2	2
1999CAL/BRO	298.1	1	1.00	#	0.748	3.04−1	0.75	−3.04−1	−1
2005DOM/MAR	281.1–330.1	24	0.50	#	0.267	5.64−2	0.13	1.11−3	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1982VAS/PET	(4.71−1, 0.91, 2.79−1, 5)	1982VAS/PET	(7.61−1, 1.36, 7.49−1, 4)
1986NAZ/BAS2	(1.37, 2.77, −5.15−1, −1)		

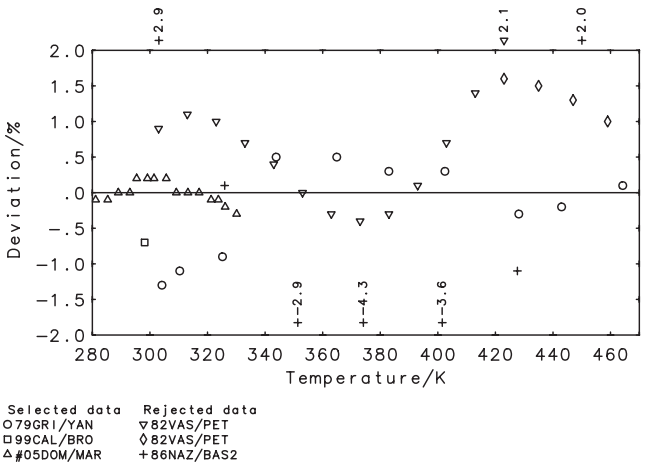

FIG. 101. Deviation plot for 1-nonanol (42-084).

Parameters of cubic spline polynomials (42.84.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	62	33	0.390	1.39−1	0.30	−2.49−3	2

T/K	A_1	A_2	A_3	A_4	Uncert.
281.1–380.0	2.534 61+2	−2.199 31+2	7.141 59+1	−7.230 03	III
380.0–464.2	−4.501 76+2	3.355 71+2	−7.476 90+1	5.59320	IV

Parameters of quasipolynomial equation (42.84.4)

Type	nTot	nPts	sw	s/R	sr/%	sb/R	+/−
C	62	33	0.371	1.35−1	0.29	6.32−3	9

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
281.1–464.2	671.50	1.292 76+4	1.528 38+3	−1.559 35+3	1.217 23+4	1.739 15+3	7.910 24+3	IV

Deviation plot for 1–Nonanol (42–084) is given in Fig. 101.

6.5.2.32. 2-Naphthol (42-086)

Name:	2-Naphthol
Formula:	$C_{10}H_8O$
CAS-RN:	135-19-3
Group No:	42-086

Experimental heat capacities (42.86.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1926AND/LYN	N	394.0–478.0	eqn	n/a	n/a		p	DSIO	1926AND/LYN
2003ROJ/ORO		397.0–416.0	21	n/a	99.94	melpt	p	BDHT	1995DIO/MAN

Reference	Notes
1926AND/LYN	calculated from temperature dependence of enthalpy by the compilers

6.5.2.33. 1-Decanol (42-090)

Name:	1-Decanol
Formula:	$C_{10}H_{22}O$
CAS-RN:	112-30-1
Group No:	42-090

Experimental heat capacities (42.90.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1967GRA		308.1–338.1	4	1.00	n/a		*p*	BSIO	1967GRA
1975WOY/KAL		303.1	1	n/a	n/a		*p*	BSIO	1970REC
1979GRI/YAN		305.8–463.3	9	0.90	n/a		*p*	BDAO	1975RAS/GRI
1979SVE		301.0-461.0	33 S	n/a	99.80	chrom	sat	BDHT	1969PER/COM
1980VAS/TRE	323.0–403.0	eqn		2.00	99.2	anal	sat	BSAO	1980VAS/TRE
1980VAS/TRE		403.0–503.0	eqn	2.00	99.2	anal	sat	BSAO	1980VAS/TRE
1985COS/PAT8		283.1–313.1	3	n/a	99.	estim	*p*	FSIT	1971PIC/LED
1988AND/PAT	298.1		1	n/a	98.	anal	*p*	FSIT	1971PIC/LED
1988NAZ/BAS		304.0–523.0	9	2.20	99.1	anal	*p*	BDHO	1986NAZ/BAS1
1992PFE/SCH		298.1–313.1	2	n/a	n/a		*p*	BDCT	1968WAD
1998RUZ/MAJ	N	304.4–404.7	38	1.00	99.70	chrom	*p*	BDCT	1991BAN/GAR
1999CAL/BRO		298.1	1	n/a	99.0	chrom	*p*	FSIT	1971PIC/LED
2000FUL/RUZ		330.6–570.7	13	2.00	99.87	chrom	sat	BDCT	1991BAN/GAR
2003VAN/GAB		282.9–388.1	50	0.20	99.78	melpt	*p*	BSAO	1998VAN/VAN
2005DOM/MAR		284.2–308.1	24	n/a	99.0	chrom	*p*	BDCT	1989BRE/LIC
2006DZI/GOR		290.9–318.4	30	0.15	99.0	anal	*p*	BDCT	2000ERN/CHO

Reference	Notes
1998RUZ/MAJ	same data in 2004RUZ/FUL

Correlated heat capacities (42.90.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1975WOY/KAL	303.1	1	0.50	#	0.499	1.13−1	0.25	−1.13−1	−1
1979SVE	301.0–461.0	33	3.00	#	0.080	1.28−1	0.24	−4.92−2	−12
1980VAS/TRE	403.0–502.9	10	2.00		0.317	3.79−1	0.63	3.44−1	10
1988AND/PAT	298.1	1	0.50	#	0.238	5.34−2	0.12	5.34−2	1
1998RUZ/MAJ	304.4–404.7	38	1.00		0.397	1.98−1	0.40	−1.87−1	−38
1999CAL/BRO	298.1	1	0.50	#	0.731	1.63−1	0.37	−1.63−1	−1
2000FUL/RUZ	330.6–570.7	13	2.00		0.289	3.41−1	0.58	−2.38−1	−11
2003VAN/GAB	282.9–388.1	50	1.00	#	0.347	1.69−1	0.35	1.61−1	48
2005DOM/MAR	284.2–308.1	24	1.00	#	0.178	7.86−2	0.18	−2.12−2	−5
2006DZI/GOR	290.9–318.4	30	0.15		0.282	1.92−2	0.04	5.62−4	5

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1967GRA	(1.75, 3.88, −1.63, −4)	1979GRI/YAN	(7.90−1, 1.37, 5.90−1, 5)
1980VAS/TRE	(6.22−1, 1.21, −5.28−1, −8)	1985COS/PAT8	(4.34−1, 1.00, −4.09−1, −3)
1988NAZ/BAS	(3.12, 4.84, 1.15, −1)	1992PFE/SCH	(2.11, 4.41, 2.11, 2)

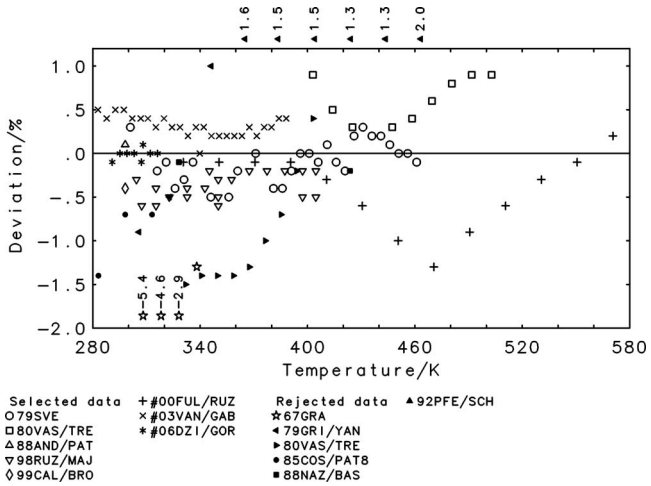

FIG. 102. Deviation plot for 1-decanol (42-090).

Parameters of cubic spline polynomials (42.90.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	238	201	0.306	1.84−1	0.35	−5.32−3	−4
sat	238	201	0.307	1.86−1	0.35	−5.34−3	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
282.9–375.0	2.610 39+2	−2.240 49+2	7.282 26+1	−7.37927	II
375.0–450.0	−2.988 60+2	2.238 71+2	−4.662 26+1	3.238 08	II
450.0–570.7	−2.429 62+2	1.866 05+2	−3.834 14+1	2.624 66	IV
282.9–375.0	2.609 36+2	−2.239 53+2	7.279 32+1	−7.376 27	II
375.0–450.0	−2.981 57+2	2.233 21+2	−4.648 00+1	3.225 79	II
450.0–570.7	−2.335 22+2	1.802 31+2	−3.690 44+1	2.516 48	IV

Deviation plot for 1–Decanol (42–090) is given in Fig. 102.

6.5.2.34. 1-Undecanol (42-094)

Name:	1-Undecanol
Formula:	$C_{11}H_{24}O$
CAS-RN:	112-42-5
Group No:	42-094

Experimental heat capacities (42.94.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1982VAS/PET		303.0–433.0	eqn	n/a	99.7	anal	sat	BSAO	1980VAS/TRE
1982VAS/PET		433.0–523.0	eqn	n/a	99.7	anal	sat	BSAO	1980VAS/TRE
1987NAZ/BAD		303.6–499.6	9	n/a	n/a		p	BDHO	1986NAZ/BAS1
1988AND/PAT		298.1	1	n/a	98.	anal	p	FSIT	1971PIC/LED
2005DOM/MAR		297.1–323.3	24	n/a	98.0	chrom	p	BDCT	1989BRE/LIC

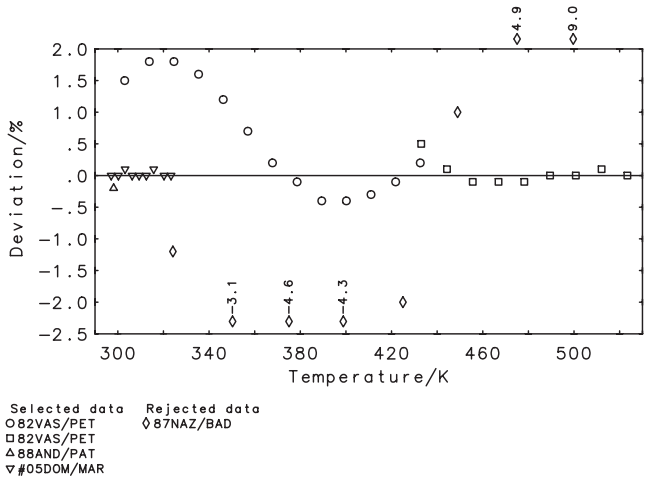

FIG. 103. Deviation plot for 1-undecanol (42-094).

Correlated heat capacities (42.94.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1982VAS/PET	346.2–432.6	9	3.00	#	0.169	2.97−1	0.51	6.20−2	−1
1982VAS/PET	433.0–523.4	9	3.00	#	0.063	1.23−1	0.19	2.63−2	0
1988AND/PAT	298.1	1	0.50	#	0.483	1.18−1	0.24	−1.18−1	−1
2005DOM/MAR	297.1–323.3	24	0.50	#	0.115	2.89−2	0.06	4.09−3	2
	Rejected data: Reference (d/R, d_r, d_b/R, +/−)								
1987NAZ/BAD	(2.86, 4.23, 1.92−1, −1)								

Parameters of cubic spline polynomials (42.94.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	56	43	0.149	1.60−1	0.27	1.80−2	0

T/K	A_1	A_2	A_3	A_4	Uncert.
297.1–390.0	2.025 96+2	−1.669 89+2	5.537 06+1	−5.581 80	III
390.0–523.4	−3.307 96+2	2.433 12+2	−4.983 48+1	3.410 11	V

Deviation plot for 1–Undecanol (42–094) is given in Fig. 103.

6.5.2.35. 1-Dodecanol (42-095)

Name:	1-Dodecanol
Formula:	$C_{12}H_{26}O$
CAS-RN:	112-53-8
Group No:	42-095

Experimental heat capacities (42.95.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1979SVE		316.0–486.0	35	S	n/a	99.98	chrom	sat	BDHT	1969PER/COM
1982VAS/PET		303.0–423.0	eqn		n/a	99.9	anal	sat	BSAO	1980VAS/TRE
1982VAS/PET		423.0–533.0	eqn		n/a	99.9	anal	sat	BSAO	1980VAS/TRE
1988AND/PAT		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1998RUZ/MAJ	N	307.2–357.6	24		1.00	99.00	chrom	*p*	BDCT	1991BAN/GAR

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003VAN/VAN1		301.5–390.5	32	0.20	98.0	anal	p	BSAO	1998VAN/VAN

Reference	Notes
1998RUZ/MAJ	same data in 2004RUZ/FUL

Correlated heat capacities (42.95.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979SVE	316.0–486.0	35	1.50	#	0.117	1.13−1	0.18	−3.60−2	−12
1988AND/PAT	298.1	1	1.00	#	0.510	2.69−1	0.51	−2.69−1	−1
1998RUZ/MAJ	307.2–357.6	24	1.00		0.333	1.84−1	0.33	−1.51−1	−24
2003VAN/VAN1	301.5–390.5	30	0.20		0.113	1.33−2	0.02	6.00−3	10

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1982VAS/PET	(2.54, 3.93, 2.52, 12)	1982VAS/PET	(2.60, 3.67, 2.60, 6)

Parameters of cubic spline polynomials (42.95.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	115	90	0.211	1.26−1	0.22	−5.53−2	−27
sat	115	90	0.211	1.26−1	0.22	−5.53−2	−28

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–380.0	3.082 82+2	−2.581 96+2	8.258 02+1	−8.283 99	III
380.0–486.0	−4.131 38+2	3.113 47+2	−6.729 95+1	4.863 34	IV
298.1–380.0	3.081 36+2	−2.580 67+2	8.254 24+1	−8.280 31	III
380.0–486.0	−4.125 65+2	3.109 08+2	−6.718 78+1	4.853 92	IV

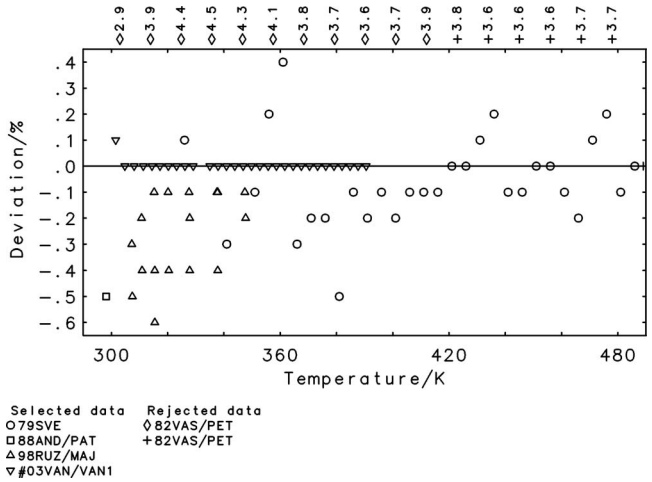

FIG. 104. Deviation plot for 1-dodecanol (42-095).

Parameters of quasipolynomial equation (42.95.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	115	90	0.874	1.71−1	0.30	−4.44−2	−27

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
298.1–486.0	720.00	4.887 69+3	6.608 94+2	−6.405 56+2	4.229 72+3	1.854 71+3	1.525 20+3	IV

Deviation plot for 1–Dodecanol (42–095) is given in Fig. 104.

6.5.2.36. 1-Tridecanol (42-097)

Name:	1-Tridecanol
Formula:	$C_{13}H_{28}O$
CAS-RN:	112-70-9
Group No:	42-097

Experimental heat capacities (42.97.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1974MOS/MOU		305.0–346.0	eqn	n/a	99.97	chrom	p	BSAO	1974MOS/MOU
1977BEL/BUB		313.1	1	n/a	n/a		p	BDCT	1968WAD
1980VAS/TRE		323.0–423.0	eqn	2.00	99.2	anal	sat	BSAO	1980VAS/TRE
1980VAS/TRE		423.0–553.0	eqn	2.00	99.2	anal	sat	BSAO	1980VAS/TRE
2003VAN/VAN1		307.0–369.1	40	0.20	98.0	anal	p	BSAO	1998VAN/VAN

6.5.2.37. 1-Pentadecanol (42-101)

Name:	1-Pentadecanol
Formula:	$C_{15}H_{32}O$
CAS-RN:	629-76-5
Group No:	42-101

Experimental heat capacities (42.101.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1974MOS/MOU		318.0–346.0	eqn	n/a	99.97	chrom	p	BSAO	1974MOS/MOU
1982VAS/PET		333.0–413.0	eqn	n/a	99.4	anal	sat	BSAO	1980VAS/TRE
1982VAS/PET		413.0–513.0	eqn	n/a	99.4	anal	sat	BSAO	1980VAS/TRE
1982VAS/PET		513.0–583.0	eqn	n/a	99.4	anal	sat	BSAO	1980VAS/TRE
2003VAN/VAN1		318.4–380.0	60	0.50	98.0	anal	p	BSAO	1998VAN/VAN

Correlated heat capacities (42.101.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2003VAN/VAN1	318.4–380.0	60	0.50	0.263	9.43−2	0.13	2.32−4	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1974MOS/MOU	(2.55, 3.70, −2.53, −9)	1982VAS/PET	(1.88, 2.56, −1.84, −6)

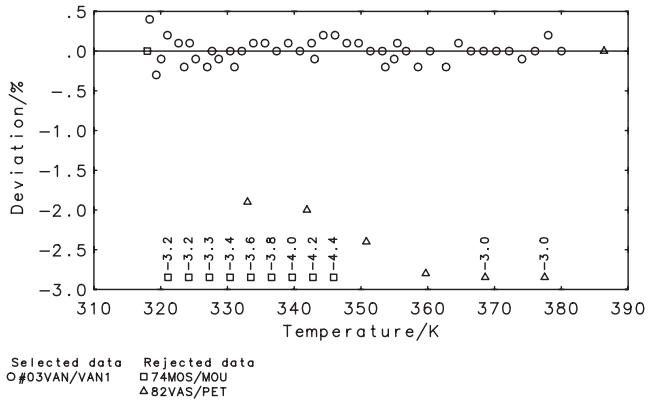

FIG. 105. Deviation plot for 1-pentadecanol (42-101).

Parameters of regression polynomial (42.101.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	100	60	0.272	9.76−2	0.14	2.32−4	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
318.4–380.0	9.844 27+2	−8.227 89+2	2.421 84+2	−2.326 57+1	II

Parameters of quasi-polynomial equation (42.101.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	100	60	0.290	1.04−1	0.14	−2.24−2	−16

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
318.4–380.0	759.00	3.668 67+5	4.904 99+4	−5.111 55+4	3.391 75+5	5.671 59+4	1.889 62+5	II

Deviation plot for 1–Pentadecanol (42–101) is given in Fig. 105.

6.5.2.38. 1-Hexadecanol (42-102)

Name:	1-Hexadecanol
Formula:	$C_{16}H_{34}O$
CAS-RN:	36653-82-4
Group No:	42-102

Experimental heat capacities (42.102.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1974MOS/MOU		323.0–346.0	eqn	n/a	99.96	chrom	p	BSAO	1974MOS/MOU
1998RUZ/MAJ	N	327.6–387.2	35	1.00	99.60	chrom	p	BDCT	1991BAN/GAR

Reference	Notes
1998RUZ/MAJ	same data in 2004RUZ/FUL

6.5.2.39. 1-Octadecanol (42-103)

Name:	1-Octadecanol
Formula:	$C_{18}H_{38}O$
CAS-RN:	112-92-5
Group No:	42-103

Experimental heat capacities (42.103.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1980VAS/TRE		353.0–413.0	eqn	2.00	99.8	anal	sat	BSAO	1980VAS/TRE
1980VAS/TRE		413.0–513.0	eqn	2.00	99.8	anal	sat	BSAO	1980VAS/TRE
1980VAS/TRE		513.0–623.0	eqn	2.00	99.8	anal	sat	BSAO	1980VAS/TRE
1998RUZ/MAJ	N	337.6–397.2	28	1.00	99.60	chrom	*p*	BDCT	1991BAN/GAR
2001VAN/OON2		332.6–358.7	18	0.20	98.0	anal	*p*	BSAO	1987VAN/VAN

Reference	Notes
1998RUZ/MAJ	same data in 2004RUZ/FUL

6.5.2.40. (±)-1,2-Butanediol (42-108)

Name:	(±)-1,2-Butanediol
Formula:	$C_4H_{10}O_2$
CAS-RN:	26171-83-5
Group No:	42-108

Experimental heat capacities (42.108.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996STE/CHI1		300.0–670.0	20	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
1998HAW/GRA		298.1	1		n/a	99.0	chrom	*p*	BSIO	1998HAW/GRA

6.5.2.41. 2,2-Dimethyl-1-propanol (42-109)

Name:	2,2-Dimethyl-1-propanol
Formula:	$C_5H_{12}O$
CAS-RN:	75-84-3
Group No:	42-109

Experimental heat capacities (42.109.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997CEN/RUZ		335.4–362.6	10	1.00	99.79	chrom	*p*	BDCT	1991BAN/GAR
2003CEN/RUZ	N	335.2–360.1	8	1.00	n/a		*p*	BDCT	1991BAN/GAR
2007STR/VAN		331.6–361.9	31	0.20	99.79	chrom	*p*	BSAO	1998VAN/VAN

Reference	Notes
2003CEN/RUZ	same data in 1997CEN/RUZ

6.5.2.42. 1-Methylcyclopentanol (42-110)

Name:	1-Methylcyclopentanol
Formula:	$C_6H_{12}O$
CAS-RN:	1462-03-9
Group No:	42-110

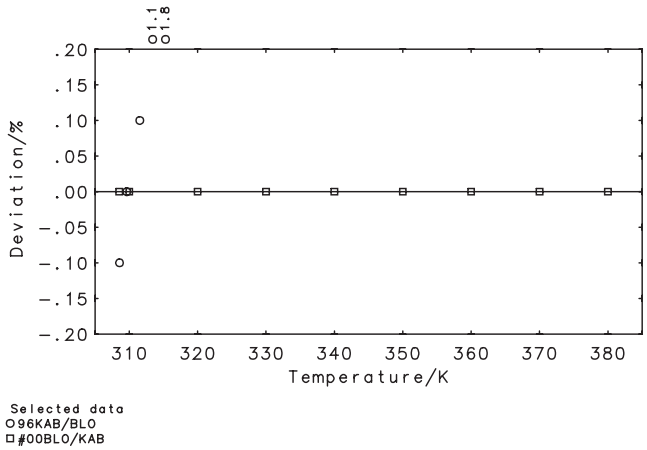

FIG. 106. Deviation plot for 1-methylcyclopentanol (42-110).

Experimental heat capacities (42.110.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996KAB/BLO		308.6–315.3	5		0.40	99.96	chrom	sat	BSAO	1993DIK/KAB
2000BLO/KAB	N	308.5–380.0	9	S	2.00	99.96	chrom	p	BDHT	1992KAB/KOZ

Reference	Notes
2000BLO/KAB	smoothed in this paper

Correlated heat capacities (42.110.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1996KAB/BLO	308.6–311.5	3	0.40	0.232	2.79−2	0.09	1.05−3	1
2000BLO/KAB	308.5–380.0	9	2.00	0.014	9.09−3	0.03	−8.38−3	−8

Parameters of regression polynomial (42.110.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	14	12	0.128	1.76−2	0.06	−6.02−3	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
308.5–380.0	1.715 90+1	4.166 52			III

Deviation plot for 1–Methylcyclopentanol (42–110) is given in Fig. 106.

6.5.2.43. 1,6-Hexanediol (42-111)

Name:	1,6-Hexanediol
Formula:	$C_6H_{14}O_2$
CAS-RN:	629-11-8
Group No:	42-111

Experimental heat capacities (42.111.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991STE/CHI2		333.0–513.0	10	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2005SMI/KAN		317.3–370.0	20	0.20	99.05	melpt	p	BSAO	1997VAR/DRU1

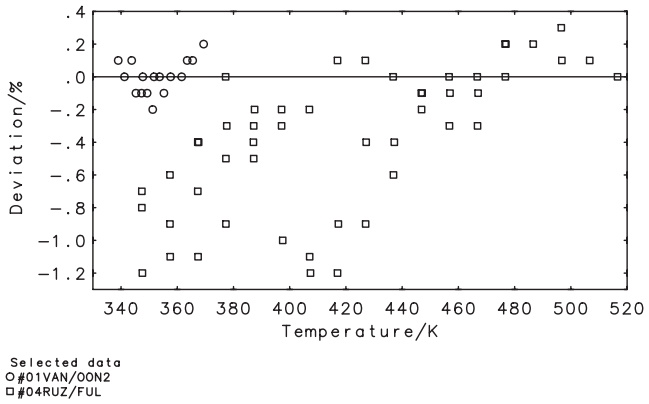

FIG. 107. Deviation plot for 1-eicosanol (42-122).

6.5.2.44. 1-Eicosanol (42-122)

Name:	1-Eicosanol
Formula:	$C_{20}H_{42}O$
CAS-RN:	629-96-9
Group No:	42-122

Experimental heat capacities (42.122.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001VAN/OON2		339.0–371.3	26	0.20	98.0	anal	p	BSAO	1987VAN/VAN
2004RUZ/FUL		347.4–516.6	52	2.00	98.5	chrom	sat	BDCT	1991BAN/GAR

Correlated heat capacities (42.122.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2001VAN/OON2	339.0–371.3	26	0.20	0.512	9.87−2	0.10	7.54−3	−3
2004RUZ/FUL	347.4–516.6	52	2.00	0.283	5.58−1	0.57	−3.58−1	−24

Parameters of regression polynomial (42.122.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	78	78	0.385	4.71−1	0.48	−2.36−1	−27	
T/K		A_1		A_2		A_3	A_4	Uncert.
339.0–516.6		−4.244 10+2		3.513 23+2		−7.855 53+1	5.895 21	III

Deviation plot for 1–Eicosanol (42–122) is given in Fig. 107.

6.5.2.45. 1,3-Propanediol (42-126)

Name:	1,3-Propanediol
Formula:	$C_3H_8O_2$
CAS-RN:	504-63-2
Group No:	42-126

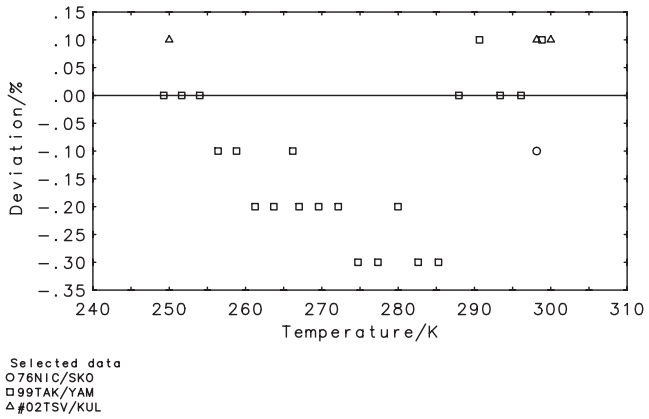

FIG. 108. Deviation plot for 1,3-propanediol (42-126).

Experimental heat capacities (42.126.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1976NIC/SKO		298.1	1		0.20	n/a		p	DDCT	1971KON/SUU
1999TAK/YAM		249.3–298.9	21		n/a	n/a		p	BSAO	1987YAM/OGU
2002TSV/KUL		250.0–300.0	3	S	0.20	n/a		p	BSAO	1997VAR/DRU1

Correlated heat capacities (42.126.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1976NIC/SKO	298.1	1	0.20		0.536	2.27−2	0.11	−2.27−2	−1
1999TAK/YAM	249.3–298.9	21	1.00	#	0.182	3.65−2	0.18	−2.49−2	−16
2002TSV/KUL	250.0–300.0	3	0.20		0.361	1.50−2	0.07	1.47−2	3

Parameters of regression polynomial (42.126.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	25	25	0.244	3.56−2	0.18	−2.01−2	−14

T/K	A_1	A_2	A_3	A_4	Uncert.
249.3–300.0	6.653 17	4.892 03			I

Deviation plot for 1,3–Propanediol (42–126) is given in Fig. 108.

6.5.2.46. 2,6-Dimethylphenol (42-127)

Name:	2,6-Dimethylphenol
Formula:	$C_8H_{10}O$
CAS-RN:	576-26-1
Group No:	42-127

Experimental heat capacities (42.127.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996LEB/VAS		318.7–600.0	4	S	2.50	99.904	melpt	p	BDHT	1985GUS/DAV

Parameters of regression polynomial (42.127.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.006	5.78−3	0.02	−7.34−5	0
T/K		A_1		A_2	A_3	A_4	Uncert.
318.7–600.0		1.061 24+1		5.169 88			V

6.5.2.47. α-Methylbenzenemethanol (42-128)

Name:	α-Methylbenzenemethanol
Formula:	$C_8H_{10}O$
CAS-RN:	98-85-1
Group No:	42-128

Experimental heat capacities (42.128.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001BEC/GME		310.1–360.0	11	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Parameters of regression polynomial (42.128.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
sat	11	11	0.234	3.96−2	0.12	6.59−5	1	
T/K		A_1		A_2		A_3	A_4	Uncert.
310.1–360.0		−4.818 91+1		4.296 67+1		−5.504 43		II

6.5.2.48. 2,2,4-Trimethyl-1,3-pentanediol (42-129)

Name:	2,2,4-Trimethyl-1,3-pentanediol
Formula:	$C_8H_{18}O_2$
CAS-RN:	144-19-4
Group No:	42-129

Experimental heat capacities (42.129.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI2		350.0–450.0	6	S	n/a	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (42.129.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
sat	6	6	0.107	2.80−2	0.05	1.33−5	1	
T/K		A_1		A_2		A_3	A_4	Uncert.
350.0–450.0		−4.302 48+1		3.961 06+1		−3.976 33		II

6.5.2.49. 2-Butyl-2-ethyl-1,3-propanediol (42-130)

Name:	2-Butyl-2-ethyl-1,3-propanediol
Formula:	$C_9H_{20}O_2$
CAS-RN:	115-84-4
Group No:	42-130

Experimental heat capacities (42.130.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI2		340.0–500.0	9	S	n/a	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (42.130.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
sat	9	9	0.470	1.36−1	0.23	3.84−4	1	
T/K		A_1		A_2		A_3	A_4	Uncert.
340.0–500.0		−9.899 87		2.551 29+1		−2.217 69		II

6.5.2.50. Tricyclo[3.3.1.1^{3,7}]decan-1-ol (42-131)

Name:	Tricyclo[3.3.1.1^{3,7}]decan-1-ol
Formula:	$C_{10}H_{16}O$
CAS-RN:	768-95-6
Group No:	42-131

Experimental heat capacities (42.131.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003CHA/BLO		598.0–610.0	eqn	2.00	99.98	chrom	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (42.131.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	3	3	0.000	3.82−6	0.00	1.27−6	0
T/K		A_1		A_2	A_3	A_4	Uncert.
598.0–610.0		1.865 40+1		5.255 93			V

6.5.2.51. Tricyclo[3.3.1.1^{3,7}]decan-2-ol (42-132)

Name:	Tricyclo[3.3.1.1^{3,7}]decan-2-ol
Formula:	$C_{10}H_{16}O$
CAS-RN:	700-57-2
Group No:	42-132

Experimental heat capacities (42.132.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003CHA/BLO		567.0–610.0	eqn	2.00	99.93	chrom	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (42.132.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	5	5	0.000	3.82−6	0.00	−7.63−7	0
T/K		A_1		A_2	A_3	A_4	Uncert.
567.0–610.2		2.940 66+1		3.872 77			V

6.5.2.52. 5-Methyl-5-nonanol (42-133)

Name:	5-Methyl-5-nonanol
Formula:	$C_{10}H_{22}O$
CAS-RN:	33933-78-7
Group No:	42-133

Experimental heat capacities (42.133.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004CER/GON	N	278.1–68.1	19	n/a	97.0	anal	p	BDHT	1969PER/COM
Reference	Notes								
2004CER/GON	data in supporting information								

Parameters of regression polynomial (42.133.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	19	19	0.436	1.09−1	0.22	4.58−4	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
278.1-368.1		−.432 10+1		3.499 27+1		−2.707 40		II

6.5.2.53. 2-Methyltricyclo[3.3.1.1^{3,7}]decan-2-ol (42-134)

Name:	2-Methyltricyclo[3.3.1.1^{3,7}]decan-2-ol
Formula:	$C_{11}H_{18}O$
CAS-RN:	702-98-7
Group No:	42-134

Experimental heat capacities (42.134.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002CHA/BLO		489.0–530.0	eqn	2.00	99.94	chrom	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (42.134.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	10	10	0.000	3.30−6	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
489.0–530.4		2.645 98+1		4.356 27			III

6.5.2.54. 9*H*-Fluorene-9-methanol (42-135)

Name:	9*H*-Fluorene-9-methanol
Formula:	$C_{14}H_{12}O$
CAS-RN:	24324-17-2
Group No:	42-135

Experimental heat capacities (42.135.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004DI/TAN		378.4–389.7	7	0.30	99.9	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (42.135.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.491	7.90−2	0.15	7.36−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
378.4–389.7	−9.625 92+2	4.822 17+2	−5.670 61+1		II

6.5.2.55. 1-Heptadecanol (42-136)

Name:	1-Heptadecanol
Formula:	$C_{17}H_{36}O$
CAS-RN:	1454-85-9
Group No:	42-136

Experimental heat capacities (42.136.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003VAN/VAN1		331.1–368.8	30	0.50	98.0	anal	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (42.136.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	30	30	0.511	2.05−1	0.26	9.69−4	5

T/K	A_1	A_2	A_3	A_4	Uncert.
331.1–368.8	2.022 00+1	1.766 28+1			III

6.5.3. Sub group 43: carbonyl compounds

6.5.3.1. 2-Butanone (43-007)

Name:	2-Butanone
Formula:	C_4H_8O
CAS-RN:	78-93-3
Group No:	43-007

Experimental heat capacities (43.7.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1933KOL/UDO	N	297.0	1		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1938PAN/DUD	N	298.0–363.0	eqn		n/a	n/a	n/a	*p*	n/a	n/a
1956PAR/KEN		180.0–300.0	13	S	1.00	99.7	melpt	*p*	BSIO	1925PAR
1964SIN/OET		191.6–336.4	64		0.30	99.78	melpt	sat	BSAO	1958HIL/KRA
1967RAS/GAN		293.1–353.1	4	S	0.50	n/a	n/a	*p*	BSAO	1967RAS/GAN
1968AND/COU2		190.8–319.8	27		n/a	99.98	melpt	sat	BSAO	1963AND/COU1
1975GRO/BEN		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1978ROU/PER1		283.1–313.1	3	S	0.30	99.8	chrom	*p*	FSIT	1971PIC/LED
1980FUC		298.2	1		0.50	n/a	n/a	*p*	BSIO	1980FUC
1984GRO/BEN		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1985COS/PAT9		283.1–313.1	3		n/a	99.	chrom	*p*	FSIT	1971PIC/LED
1991KAL/KOH		293.1–313.1	2		1.00	99.89	anal	*p*	FSIT	1971PIC/LED
1997HOV/ROU		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
2001TAM		298.1	1		n/a	99.9	chrom	*p*	FSIO	1985OGA

Reference	Notes
1933KOL/UDO	same datum in 1934KOL/UDO2
1938PAN/DUD	temperature range of parameters validity estimated by the compilers

Correlated heat capacities (43.7.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1964SIN/OET	191.6–336.4	64	0.30		0.571	3.18−2	0.17	4.87−3	8
1967RAS/GAN	293.1–353.1	4	0.50		0.899	9.02−2	0.45	−6.47−2	−4
1968AND/COU2	190.8–319.8	27	0.20	#	0.318	1.17−2	0.06	−3.75−3	−12
1997HOV/ROU	298.1	1	0.30	#	0.116	6.62−3	0.03	6.62−3	1
2001TAM	298.1	1	1.50	#	1.019	2.96−1	1.53	2.96−1	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1933KOL/UDO	(2.70−1, 1.40, 2.70−1, 1)	1938PAN/DUD	(1.40, 7.39, −1.47−1, −1)
1956PAR/KEN	(1.79−1, 0.94, 1.57−1, 11)	1975GRO/BEN	(4.75−2, 0.25, 4.75−2, 1)
1978ROU/PER1	(2.34−1, 1.26, −1.31−1, −1)	1980FUC	(1.22−1, 0.64, −1.22−1, −1)
1984GRO/BEN	(1.08−1, 0.57, −1.08−1, −1)	1985COS/PAT9	(2.34−1, 1.26, −1.31−1, −1)
1991KAL/KOH	(1.59−1, 0.83, 1.19−2, 0)		

Parameters of regression polynomial (43.7.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	128	97	0.548	4.51−2	0.23	2.63−3	−6
sat	128	97	0.549	4.52−2	0.24	2.60−3	−8

T/K	A_1	A_2	A_3	A_4	Uncert.
190.8–353.1	1.894 52+1	−1.369 88	3.742 49−1	3.441 46−2	II
190.8–353.1	1.923 69+1	−1.734 77	5.244 79−1	1.405 35−2	II

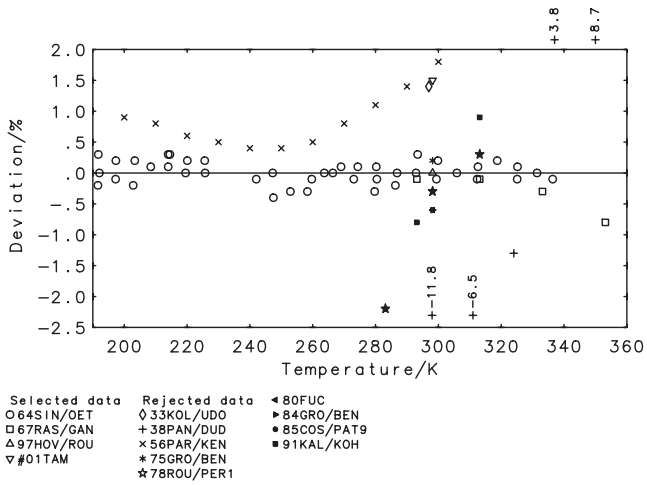

FIG. 109. Deviation plot for 2-butanone (43-007).

Parameters of quasipolynomial equation (43.7.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	128	97	0.554	4.26−2	0.22	−2.60−3	−11

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
190.8–353.1	536.78	4.442 43+1	2.854 04	1.451 75+1	4.814 64+1	−1.227 03+1	6.554 86+1	II

Deviation plot for 2–Butanone (43–007) is given in Fig. 109.

6.5.3.2. Cyclopentanone (43-008)

Name:	Cyclopentanone
Formula:	C_5H_8O
CAS-RN:	120-92-3
Group No:	43-008

Experimental heat capacities (43.8.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1980FUC		298.2	1	0.50	n/a	n/a	p	BSIO	1980FUC
1987SHV/PES		217.8–327.5	29	n/a	n/a	n/a	p	BSAO	1978ZHU/ATR
1997HOV/ROU		298.1	1	n/a	99.	chrom	p	FSIT	1971PIC/LED
2002BRO/PIN		298.1	1	n/a	99.0	chrom	p	FSIT	1971PIC/LED

6.5.3.3. 2-Pentanone (43-013)

Name:	2-Pentanone
Formula:	$C_5H_{10}O$
CAS-RN:	107-87-9
Group No:	43-013

Experimental heat capacities (43.13.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1965OET		202.0–334.0	42	0.30	99.81	melpt	sat	BSAO	1958HIL/KRA
1968AND/COU2		200.9–364.1	40	n/a	99.97	melpt	sat	BSAO	1963AND/COU1
1970HAR/HEA		298.1	1	n/a	n/a	n/a	*p*	n/a	n/a
1975GRO/BEN		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1979SAL/PEA		298.1	1	n/a	n/a	n/a	*p*	BSIO	1980FUC
1980FUC		298.2	1	0.50	n/a	n/a	*p*	BSIO	1980FUC
2002BRO/PIN		298.1	1	n/a	99.0	chrom	*p*	FSIT	1971PIC/LED

6.5.3.4. Cyclohexanone (43-017)

Name:	Cyclohexanone
Formula:	$C_6H_{10}O$
CAS-RN:	108-94-1
Group No:	43-017

Experimental heat capacities (43.17.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1924HER/BLO		289.6	1		n/a	n/a	n/a	*p*	DSIO	1922HER/SCH
1939PHI		303.9	1		n/a	n/a	n/a	*p*	BSIO	1949WEI
1971VAN		250.0–280.0	7	S	n/a	99.95	melpt	sat	BSAO	1972VAN
1980FUC		298.2–298.2	2		0.50	n/a	n/a	*p*	BSIO	1980FUC
1980NAK/SUG		244.8–301.4	25		0.30	99.92	melpt	sat	BSAO	1965SUG/SEK
1995NIS/OHO		298.1–308.1	2		n/a	99.92	chrom	*p*	FSIO	1985OGA
1997HOV/ROU		298.1	1		n/a	99.5	chrom	*p*	FSIT	1971PIC/LED

Correlated heat capacities (43.17.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1980NAK/SUG	244.8–301.4	25	0.30		0.739	4.29−2	0.22	−5.48−4	−7
1995NIS/OHO	298.1–308.1	2	1.00	#	0.513	1.10−1	0.51	5.70−2	0
1997HOV/ROU	298.1	1	1.50	#	0.659	2.12−1	0.99	2.12−1	1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1924HER/BLO	(5.21−1, 2.44, 5.21−1, 1)	1939PHI	(2.57, 10.67, 2.57, 1)
1971VAN	(1.90−1, 0.95, 1.89−1, 7)	1980FUC	(3.67−1, 1.70, 3.63−1, 2)

Parameters of regression polynomial (43.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	39	28	0.765	6.79−2	0.33	1.12−2	−6	
T/K		A_1		A_2		A_3	A_4	Uncert.
244.8–308.1		1.788 72+1		−2.434 13		1.195 16		III

Deviation plot for Cyclohexanone (43–017) is given in Fig. 110.

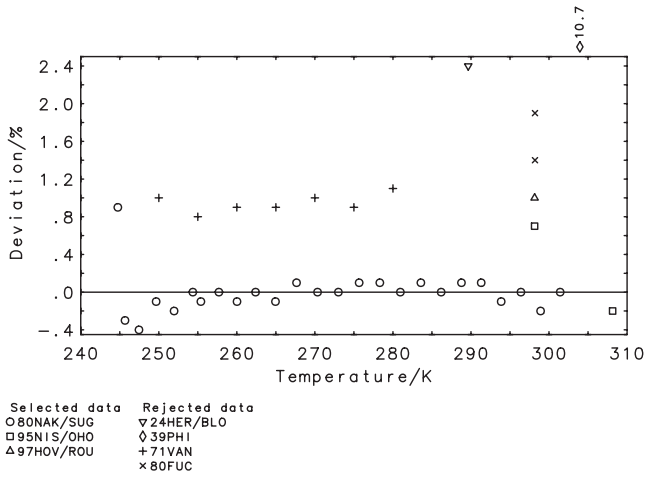

FIG. 110. Deviation plot for cyclohexanone (43-017).

6.5.3.5. 2-Heptanone (43-032)

Name:	2-Heptanone
Formula:	$C_7H_{14}O$
CAS-RN:	110-43-0
Group No:	43-032

Experimental heat capacities (43.32.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1980FUC		298.2–298.2	2	0.50	n/a	n/a	*p*	BSIO	1980FUC
2002BRO/PIN		298.1	1	n/a	98.0	chrom	*p*	FSIT	1971PIC/LED

6.5.3.6. Diphenyl methanone (43-051)

Name:	Diphenyl methanone
Formula:	$C_{13}H_{10}O$
CAS-RN:	119-61-9
Group No:	43-051

Experimental heat capacities (43.51.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1983DEK/VAN		322.5–346.6	22	n/a	99.53	melpt	*p*	BSAO	1979SCH/OFF
2002CHI/KNI2		271.4–439.7	23	0.10	99.98	melpt	sat	BSAO	1988STE/ARC
2002HAN/HIK		322.2–351.0	12	0.20	99.96	melpt	*p*	BSAO	1993FUJ/OGU1

Correlated heat capacities (43.51.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1983DEK/VAN	322.5–346.6	22	3.00	#	0.320	3.49−1	0.96	−3.49−1	−22
2002CHI/KNI2	271.4–439.7	23	0.10		0.970	3.42−2	0.10	−1.11−2	−8
2002HAN/HIK	322.2–351.0	12	0.20		1.251	9.29−2	0.25	8.97−2	12

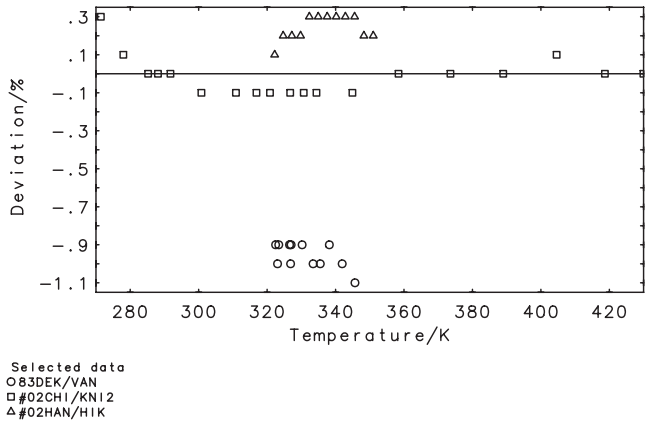

FIG. 111. Deviation plot for diphenyl methanone (43-051).

Parameters of regression polynomial (43.51.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	57	57	0.881	2.26−1	0.62	−1.20−1	−18
T/K		A_1		A_2	A_3	A_4	Uncert.
271.4–439.7		1.745 21+1		5.792 23			IV

Deviation plot for Diphenyl methanone (43–051) is given in Fig. 111.

6.5.3.7. (2*E*)-2-Butenal (43-072)

Name:	(2*E*)-2-Butenal
Formula:	C_4H_6O
CAS-RN:	123-73-9
Group No:	43-072

Experimental heat capacities (43.72.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI1		300.0–540.0	13	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of cubic spline polynomials (43.72.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
sat	13	13	0.305	7.21−2	0.30	3.45−4	0		
T/K		A_1		A_2		A_3	A_4		Uncert.
300.0–440.0		3.536 00−1		1.031 96+1		−2.202 35	2.086 79−1		II
440.0–540.0		−2.548 17+2		1.843 00+2		−4.174 33+1	3.204 20		III

Parameters of quasipolynomial equation (43.72.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−				
C	13	13	0.334	7.08−2	0.33	2.95−4	−1				
T/K		T_c/K		A_1		A_2	A_3	A_4	A_5	A_6	Uncert.
300.0–540.0		565.00		−1.891 04		1.418 87−1	1.027 96+1	1.089 71+1	−2.282 37	1.675 60−1	II

6.5.3.8. 5-Hexen-2-one (43-073)

Name:	5-Hexen-2-one
Formula:	$C_6H_{10}O$
CAS-RN:	109-49-9
Group No:	43-073

Experimental heat capacities (43.73.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI6		300.0–580.0	15	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of cubic spline polynomials (43.73.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	15	15	0.825	2.93−1	0.82	3.88−3	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
300.0–495.0	3.035 73+1	−5.246 44+1	1.079 28+2	−5.212 37+1	II
495.0–580.0	−1.627 29+3	5.915 08+3	−7.053 13+3	2.812 30+3	III

Parameters of quasipolynomial equation (43.73.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	15	15	0.161	4.89−2	0.16	1.55−4	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
300.0–580.0	594.00	−1.648 25	1.737 87−1	9.915 50	3.557 00+1	−2.120 30+1	4.615 58	III

6.5.3.9. 2-Ethylhexanal (43-074)

Name:	2-Ethylhexanal
Formula:	$C_8H_{16}O$
CAS-RN:	123-05-7
Group No:	43-074

Experimental heat capacities (43.74.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001BEC/GME		310.0–380.0	15	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Parameters of regression polynomial (43.74.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	15	15	0.274	4.76−2	0.14	1.03−4	4

T/K	A_1	A_2	A_3	A_4	Uncert.
310.0–380.0	2.644 10+1	−4.060 04−1	7.901 27−1		II

6.5.3.10. α-Methylbenzeneacetaldehyde (43-075)

Name:	α-Methylbenzeneacetaldehyde
Formula:	$C_9H_{10}O$
CAS-RN:	93-53-8
Group No:	43-075

Experimental heat capacities (43.75.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI6		293.0–513.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (43.75.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/-
sat	22	22	0.000	1.13−6	0.00	4.33−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
293.0–513.5	1.234 00+1	5.300 00			II

6.5.3.11. 2-Methyl-3-phenyl-2-propenal (43-076)

Name:	2-Methyl-3-phenyl-2-propenal
Formula:	$C_{10}H_{10}O$
CAS-RN:	101-39-3
Group No:	43-076

Experimental heat capacities (43.76.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI4		290.0–470.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (43.76.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	15	15	0.000	2.12−6	0.00	−5.09−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
290.0-470.6	1.560 00+1	5.150 00			III

6.5.3.12. Tricyclo[3.3.1.1^{3,7}]decanone (43-077)

Name:	Tricyclo[3.3.1.1^{3,7}]decanone
Formula:	$C_{10}H_{14}O$
CAS-RN:	700-58-3
Group No:	43-077

Experimental heat capacities (43.77.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004BLO/KAB	N	557.5–610.0	3	S	2.00	99.84	chrom	p	BDHT	1992KAB/KOZ

Reference	Notes
2004BLO/KAB	same data in 2006BAZ/BLO

Parameters of regression polynomial (43.77.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	3	3	0.004	3.97−3	0.01	−1.27−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
557.5–610.0	−2.851 63	8.243 35			V

6.5.4. Sub group 44: acids and anhydrides

6.5.4.1. Acetic acid (44-002)

Name:	Acetic acid
Formula:	$C_2H_4O_2$
CAS-RN:	64-19-7
Group No:	44-002

Experimental heat capacities (44.2.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		313.5–325.1	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1886LUD	N	308.1	1		n/a	n/a	n/a	avg	DSIO	1886LUD
1886SCH		312.9–337.4	8	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1895PIC	N	314.1	1		3.70	n/a	n/a	avg	BDHO	1890PIC
1900LOU	N	340.1	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1912BAU		290.1	1		n/a	n/a	n/a	p	n/a	n/a
1913NAS/BRE2		291.3–293.2	4		n/a	n/a	n/a	p	BSIO	1949WEI
1925PAR/KEL		292.6–294.7	2		n/a	99.9	estim	p	BSIO	1925PAR
1932NEU	N	297.0–353.6	4		n/a	n/a	n/a	p	BSIO	1932NEU
1934RAD/JUL		289.6	1		n/a	n/a	n/a	p	BSIO	1949WEI
1947PUS/FED		296.4–309.6	6		n/a	n/a	n/a	p	DSIO	1947PUS/FED
1958SWI/ZIE1	N	332.3-348.8	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1965CAM/GIE		298.6	1		0.50	n/a	n/a	p	DSIO	1964CAM/NAG
1981CAS/WIL		298.1	1		n/a	99.8	melpt	p	FSIT	1971PIC/LED
1982MAR/AND		293.2–350.8	30		n/a	99.95	melpt	p	BSAO	1968WES/FUR
1982MAR/AND		315.1–400.2	18		n/a	99.95	melpt	p	BSAO	1967AND/COU
1997COM/RIG		288.1–313.1	3		n/a	n/a	n/a	p	BDHT	1995DIO/MAN

Reference	Notes
1886LUD	average value in the temperature range 293−323 K
1895PIC	average value in the temperature range 290−339 K
1900LOU	average value in the temperature range 296−385 K
1932NEU	same data in 1932NEI
1958SWI/ZIE1	average values in the temperature ranges 295–369 and 295−402 K

6.5.4.2. Propanoic acid (44-004)

Name:	Propanoic acid
Formula:	$C_3H_6O_2$
CAS-RN:	79-09-4
Group No:	44-004

Experimental heat capacities (44.4.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886LUD	N	309.1	1	n/a	n/a	n/a	avg	DSIO	1886LUD
1902LOU2	N	351.7	1	n/a	n/a	n/a	avg	DSIO	1898LOU
1934RAD/JUL		289.1	1	n/a	n/a	n/a	*p*	BSIO	1949WEI
1971KON/WAD		298.1	1	n/a	99.80	melpt	*p*	BSIO	1970LKB/COM
1978WOY/KAL		303.1	1	n/a	n/a	n/a	*p*	BSIO	1970REC
1981CAS/WIL		298.1	1	n/a	99.5	melpt	*p*	FSIT	1971PIC/LED
1982BIR/SIK		270.0–370.0	eqn	1.00	n/a	n/a	*p*	BDHT	1969PER/COM
1982MAR/AND		254.8–353.1	49	n/a	99.93	melpt	*p*	BSAO	1968WES/FUR
1982MAR/AND		303.4–447.1	25	n/a	99.93	melpt	*p*	BSAO	1967AND/COU
1997COM/RIG		288.1–313.1	3	n/a	n/a	n/a	*p*	BDHT	1995DIO/MAN

Reference	Notes
1886LUD	average value in the temperature range 295–323 K
1902LOU2	average value in the temperature range 294–410 K

6.5.4.3. 2,2-Dimethylpropanoic acid (44-037)

Name:	2,2-Dimethylpropanoic acid
Formula:	$C_5H_{10}O_2$
CAS-RN:	75-98-9
Group No:	44-037

Experimental heat capacities (44.37.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1990SIN/GLI	N	313.0–319.0	eqn	n/a	99.9995	melpt	*p*	BDHT	1987PER/COM
2002STE/CHI4		309.0–440.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1990SIN/GLI	model of Perkin-Elmer DSC instrument unspecified

Correlated heat capacities (44.37.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1990SIN/GLI	313.0–319.0	4	1.00	#	0.462	1.15−1	0.46	−9.77−2	−4
2002STE/CHI4	309.0–440.6	15	1.00		0.194	5.03−2	0.19	2.62−2	4

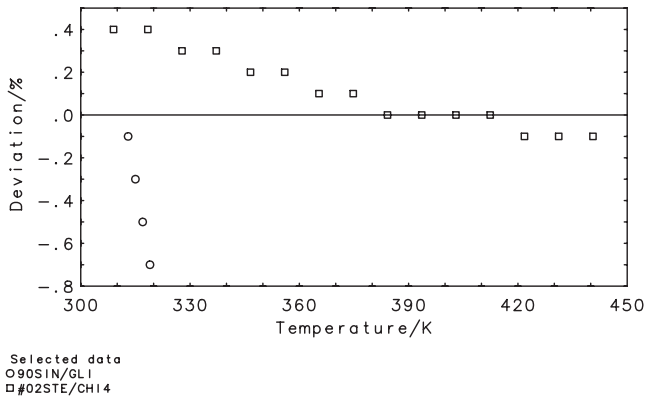

FIG. 112. Deviation plot for 2,2-dimethylpropanoic acid (44-037).

Parameters of regression polynomial (44.37.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.289	7.29−2	0.29	1.56−4	0
sat	19	19	0.289	7.29−2	0.29	1.56−4	0

T/K	A_1	A_2	A_3	A_4	Uncert.
309.0–440.6	−2.346 95−1	7.926 93			III
309.0–440.6	−2.346 95−1	7.926 93			III

Parameters of quasipolynomial equation (44.37.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.295	p	0.29	−9.45−5	−1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
309.0–440.6	633.00	−4.431 64	3.158 44−1	−6.814 71	7.177 70+1	−3.473 31+1	6.001 25	III

Deviation plot for 2,2–Dimethylpropanoic acid (44–037) is given in Fig. 112.

6.5.4.4. Cyclopropane carboxylic acid (44-040)

Name:	Cyclopropane carboxylic acid
Formula:	$C_4H_6O_2$
CAS-RN:	1759-53-1
Group No:	44-040

Experimental heat capacities (44.40.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI6		293.0–458.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (44.40.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	16	16	0.000	1.35−6	0.00	1.19−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
293.0–458.0	−1.550 00	6.000 00			III

Parameters of quasipolynomial equation (44.40.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	16	16	0.000	1.74−6	0.00	1.19−6	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
293.0–458.0	671.00	−2.742 14−4	4.66 94−10	−1.550 10	4.026 02+1	−7.388 50−4	4.519 77−9	II

6.5.4.5. Pentanedioic acid (44-041)

Name:	Pentanedioic acid
Formula:	$C_5H_8O_4$
CAS-RN:	110-94-1
Group No:	44-041

Experimental heat capacities (44.41.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI5		371.0–483.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (44.41.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	11	11	0.000	1.27−6	0.00	3.47−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
371.0–483.0	2.280 00+1	3.600 00			III

6.5.4.6. 2,2-Dimethylbutanoic acid (44-042)

Name:	2,2-Dimethylbutanoic acid
Formula:	$C_6H_{12}O_2$
CAS-RN:	595-37-9
Group No:	44-042

Experimental heat capacities (44.42.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI2		315.0–535.0	12	S	n/a	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (44.42.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.406	1.41−1	0.41	8.68−4	1
sat	12	12	0.420	7.95−2	0.21	1.80−4	0

T/K	A_1	A_2	A_3	A_4	Uncert.
315.0–535.0	1.896 09	8.621 99	−7.306 94−2		III
315.0–535.0	3.655 69+1	−1.721 17+1	6.253 16		III

Parameters of quasipolynomial equation (44.42.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.277	1.02−1	0.28	3.43−4	−2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
315.0–535.0	655.00	2.162 46+1	7.611 44−1	1.149 06+1	3.967 93+1	3.742 50+1	1.719 89+1	II

6.5.4.7. Heptanedioic acid (44-043)

Name:	Heptanedioic acid
Formula:	$C_7H_{12}O_4$
CAS-RN:	111-16-0
Group No:	44-043

Experimental heat capacities (44.43.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI5		378.0–503.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (44.43.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	13	13	0.000	1.63−6	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
378.0–502.8	2.380 00+1	5.700 00			III

6.5.4.8. 2,2-Dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid (44-044)

Name:	2,2-Dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid
Formula:	$C_{10}H_{16}O_2$
CAS-RN:	10453-89-1
Group No:	44-044

Experimental heat capacities (44.44.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004XUE/WAN		398.0–400.1	2	0.20	98.55	melpt	p	BSAO	1999TAN/ZHA

Parameters of regression polynomial (44.44.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
398.0–400.1	−1.044 80+1	1.321 67+1			II

6.5.4.9. 2,2-Dimethylpropanoic acid anhydride (44-045)

Name:	2,2-Dimethylpropanoic acid anhydride
Formula:	$C_{10}H_{18}O_3$
CAS-RN:	1538-75-6
Group No:	44-045

Experimental heat capacities (44.45.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI4		290.0–450.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (44.45.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	16	16	0.000	2.28−6	0.00	2.38−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
290.0–450.5	2.040 00+1	6.900 00			III

6.5.4.10. α-Methyl-4-(2-methylpropyl)benzeneacetic acid (44-046)

Name:	α-Methyl-4-(2-methylpropyl)benzeneacetic acid
Formula:	$C_{13}H_{18}O_2$
CAS-RN:	15687-27-1
Group No:	44-046

Experimental heat capacities (44.46.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004XU/SUN		353.4–378.8	8	0.20	99.0	anal	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (44.46.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	8	8	0.242	1.90−2	0.05	−1.24−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
353.4–378.8	4.185 90+3	−3.458 99+3	9.591 59+2	−8.842 55+1	II

6.5.5. Sub group 45: esters

6.5.5.1. Dimethyl carbonate (45-004)

Name:	Dimethyl carbonate
Formula:	$C_3H_6O_3$
CAS-RN:	616-38-6
Group No:	45-004

Experimental heat capacities (45.4.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1898LOU	N	327.0	1	n/a	n/a	n/a	avg	DSIO	1898LOU
1997STE/CHI2	N	300.0–540.0	13	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
1999PAR/TOV		288.1–308.1	3	n/a	99.	chrom	*p*	BDCT	1983ROU/ROU
2001PAR/TOV1		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2002PAR/GON		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2004DIN		278.0–323.0	eqn	n/a	n/a	n/a	*p*	BDHT	1998SAL/FER
2005PAR/TOV		288.1–308.1	3	n/a	99.0	anal	*p*	BDCT	1983ROU/ROU
2005VAL/TRO		288.1–308.1	3	n/a	99.0	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1898LOU	average value in temperature range 293–361 K
1997STE/CHI2	same data in 1997STE/CHI2

Correlated heat capacities (45.4.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1997STE/CHI2	300.0–540.0	13	1.00		0.391	9.54−2	0.39	−4.61−3	−1
1999PAR/TOV	288.1–308.1	3	0.50	#	0.304	3.02−2	0.15	2.94−2	3
2001PAR/TOV1	288.1–308.1	3	1.00	#	0.099	1.96−2	0.10	−1.15−2	−1
2002PAR/GON	288.1–308.1	3	1.00	#	0.099	1.96−2	0.10	−1.15−2	−1
2005PAR/TOV	288.1–308.1	3	1.00	#	0.099	1.96−2	0.10	−1.15−2	−1
2005VAL/TRO	288.1–308.1	3	1.00	#	0.302	6.00−2	0.30	−5.84−2	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1898LOU	(1.19−1, 0.58, 1.19−1, 1)	2004DIN	(1.98+1, >100, −1.98+1, −4)

Parameters of cubic spline polynomials (45.4.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	34	28	0.338	7.67−2	0.32	−8.96−3	−4
sat	34	28	0.282	5.99−2	0.27	−9.38−3	−4

T/K	A_1	A_2	A_3	A_4	Uncert.
288.1–490.0	2.030 33+1	−1.250 37	1.706 94−1	6.688 22−2	III
490.0–540.0	−7.466 52+3	4.582 52+3	−9.352 93+2	6.370 39+1	III
288.1–490.0	2.669 17+1	−7.005 47	1.892 78	−1.044 07−1	III
490.0–540.0	−4.655 09+3	2.859 39+3	−5.830 87+2	3.969 01+1	III

Parameters of quasipolynomial equation (45.4.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	34	28	0.584	1.05−1	0.48	1.89−2	4

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
288.1–540.0	557.00	−1.618 54	3.345 24−1	1.239 19+1	1.327 66+1	−6.398 74	1.235 12	III

Deviation plot for Dimethyl carbonate (45–004) is given in Fig. 113.

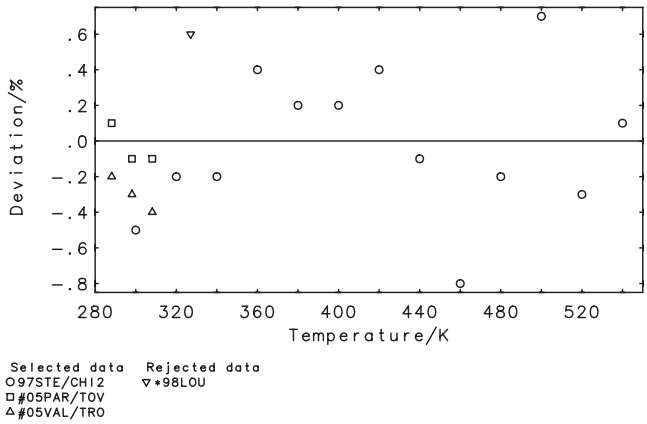

FIG. 113. Deviation plot for dimethyl carbonate (45-004).

6.5.5.2. Propyl acetate (45-018)

Name:	Propyl acetate
Formula:	$C_5H_{10}O_2$
CAS-RN:	109-60-4
Group No:	45-018

Experimental heat capacities (45.18.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		324.3–337.7	4	S	n/a	n/a	n/a	avg	DSIO	1881VON
1886SCH		307.7–322.7	6	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1986JIM/ROM		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1994JIM/ROM		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2001BEC/GME		310.1–380.0	15		0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Correlated heat capacities (45.18.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1881VON	324.3–337.7	4	2.00	#	0.712	3.56−1	1.42	3.56−1	4
1886SCH	307.7–322.7	6	2.00	#	0.997	4.92−1	1.99	4.90−1	6
1986JIM/ROM	298.1	1	0.50	#	0.108	1.27−2	0.05	1.27−2	1
1994JIM/ROM	298.1	1	0.50	#	0.291	3.44−2	0.15	3.44−2	1
2001BEC/GME	310.1–380.0	15	0.50		0.361	4.39−2	0.18	−2.05−2	−3

Parameters of regression polynomial (45.18.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	27	27	0.647	2.88−1	1.16	1.52−1	9
sat	27	27	0.646	2.87−1	1.16	1.52−1	9

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–380.0	2.171 18+1	−1.784 47	8.074 41−1		III
298.1–380.0	2.105 63+1	−1.359 36	7.386 10−1		III

Deviation plot for Propyl acetate (45–018) is given in Fig. 114.

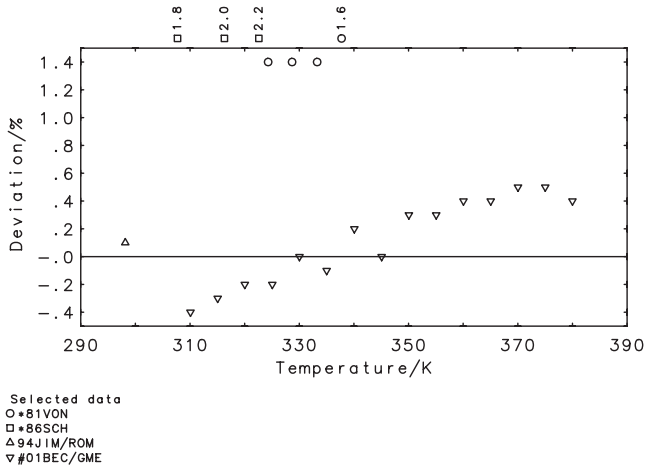

FIG. 114. Deviation plot for propyl acetate (45-018).

6.5.5.3. Diethyl carbonate (45-019)

Name:	Diethyl carbonate
Formula:	$C_5H_{10}O_3$
CAS-RN:	105-58-8
Group No:	45-019

Experimental heat capacities (45.19.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1881VON		335.6–351.4	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1898LOU	N	344.8	1		n/a	n/a	n/a	avg	DSIO	1898LOU
1934KOL/UDO2	N	294.6	1		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1999PAR/TOV		288.1–308.1	3		n/a	99.	chrom	*p*	BDCT	1983ROU/ROU
2001BEC/GME		310.0–410.1	21		0.50	99.95	chrom	sat	BDCT	2000BEC/AUF
2001PAR/TOV1		288.1–308.1	3		n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2001PAR/TOV2		288.1–308.1	3		n/a	99.0	chrom	*p*	BDHT	1969PER/COM
2004DIN		198.0–323.0	eqn		n/a	n/a	n/a	*p*	BDHT	1998SAL/FER

Reference	Notes
1898LOU	average value in the temperature range 293–396 K
1934KOL/UDO2	same datum in 1933KOL/UDO

Correlated heat capacities (45.19.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1881VON	335.6–351.4	3	3.00	#	0.340	2.89−1	1.02	1.29−1	1
1898LOU	344.8	1	5.00	#	0.066	9.26−2	0.33	9.26−2	1
1999PAR/TOV	288.1–308.1	3	0.50	#	0.366	4.86−2	0.18	9.05−3	1
2001BEC/GME	310.0–410.1	21	0.50		0.563	7.92−2	0.28	−1.53−2	3
2001PAR/TOV1	288.1–308.1	3	0.50	#	0.449	6.00−2	0.22	4.91−2	3
2001PAR/TOV2	288.1–308.1	3	0.50	#	0.449	6.00−2	0.22	4.91−2	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1934KOL/UDO2	(9.89−1, 3.90, −9.89−1, −1)	2004DIN	(2.66+1, >100, −2.66+1, −2)

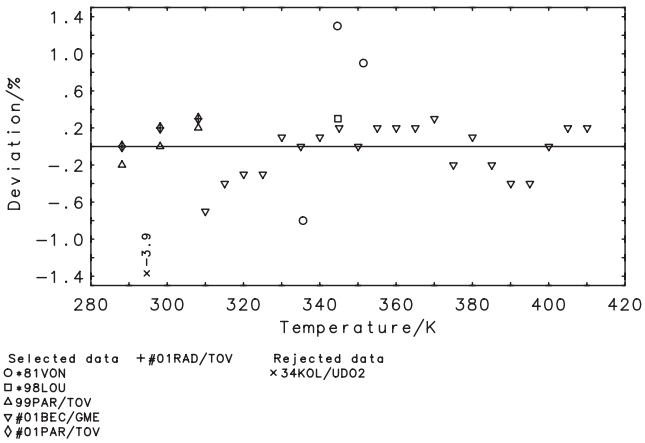

FIG. 115. Deviation plot for diethyl carbonate (45-019).

Parameters of regression polynomial (45.19.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	41	34	0.536	1.18−1	0.42	1.41−2	12

T/K	A_1	A_2	A_3	A_4	Uncert.
288.1–410.1	5.934 29+1	−3.267 22+1	9.861 28	−8.735 80−1	III

Deviation plot for Diethyl carbonate (45–019) is given in Fig. 115.

6.5.5.4. Ethyl 2,2-dimethylpropanoate (45-040)

Name:	Ethyl 2,2-dimethylpropanoate
Formula:	$C_7H_{14}O_2$
CAS-RN:	3938-95-2
Group No:	45-040

Experimental heat capacities (45.40.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1986NIL/WAD		298.1	1		n/a	99.9	chrom	*p*	DDCT	1971KON/SUU
1992VER/BEC		298.1	1		n/a	99.995	chrom	*p*	BDHT	1969PER/COM
2002STE/CHI4		300.0–540.0	13	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (45.40.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1986NIL/WAD	298.1	1	0.50	#	0.382	5.77−2	0.19	5.77−2	1
2002STE/CHI4	300.0–540.0	13	1.00		0.534	2.24−1	0.53	−1.47−2	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1992VER/BEC	(3.24, 9.71, 3.24, 1)

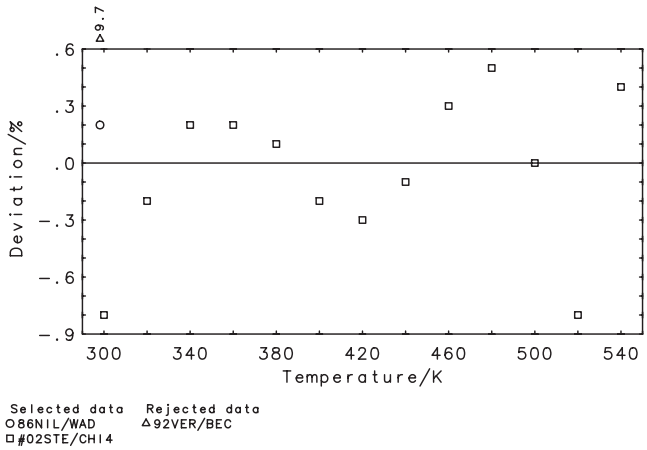

FIG. 116. Deviation plot for ethyl 2,2-dimethylpropanoate (45-040).

Parameters of cubic spline polynomials (45.40.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	15	14	0.654	2.70−1	0.64	−9.53−3	0
sat	15	14	0.498	1.85−1	0.48	−1.20−2	1

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–440.0	3.807 26+1	−1.302 19+1	4.642 98	−3.906 62−1	II
440.0–540.0	−8.884 12+2	6.186 72+2	−1.389 24+2	1.048 56+1	III
298.1–440.0	2.812 37+1	−4.972 88	2.519 95	−2.088 74−1	II
440.0–540.0	−6.225 41+2	4.386 62+2	−9.830 61+1	7.429 46	III

Parameters of quasi-polynomial equation (45.40.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	15	14	0.365	1.13−1	0.34	−1.36−2	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
298.1–540.0	566.00	−2.685 82	3.568 67−1	1.208 39+1	3.918 65+1	−2.155 66+1	4.448 21	II

Deviation plot for Ethyl 2,2–dimethylpropanoate (45–040) is given in Fig. 116.

6.5.5.5. 3-Methylbutyl acetate (45-043)

Name:	3-Methylbutyl acetate
Formula:	$C_7H_{14}O_2$
CAS-RN:	123-92-2
Group No:	45-043

Experimental heat capacities (45.43.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		307.9–332.9	6	S	n/a	n/a	n/a	avg	DSIO	1886SCH
2001BEC/GME		310.0–385.0	16		0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

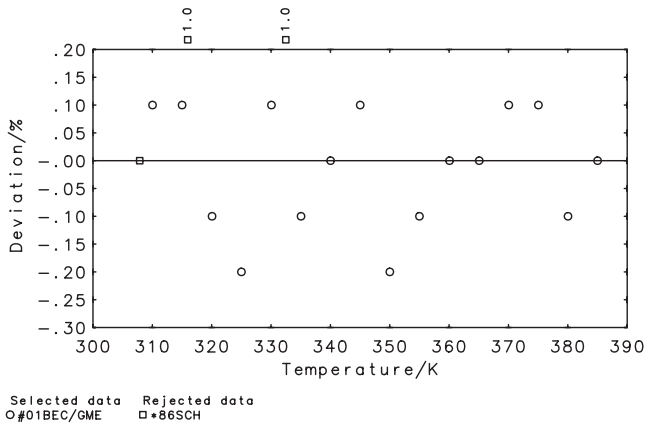

FIG. 117. Deviation plot for 3-methylbutyl acetate (45-043).

Correlated heat capacities (45.43.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2001BEC/GME	310.0–385.0	16	0.50	0.182	2.96−2	0.09	6.51−5	0
Rejected data: Reference (d/R, d_r, d_b/R, +/−)								
1886SCH	(3.24−1, 1.01, 3.24−1, 4)							

Parameters of regression polynomial (45.43.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	22	16	0.195	3.16−2	0.10	6.51−5	0
T/K		A_1		A_2	A_3	A_4	Uncert.
310.0–385.0		1.526 60+1		5.023 24			II

Deviation plot for 3–Methylbutyl acetate (45–018) is given in Fig. 117.

6.5.5.6. Methyl benzoate (45-048)

Name:	Methyl benzoate
Formula:	$C_8H_8O_2$
CAS-RN:	93-58-3
Group No:	45-048

Experimental heat capacities (45.48.1)

Reference	Note	1.526 60+1	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		317.8–345.2	6	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1971HAL/BAL	N	297.1	1		n/a	99.9	chrom	*p*	BDHT	1971DU/COM
1979FUC		298.1	1		0.50	99.0	chrom	*p*	BSIO	1980FUC
1996ROU/HER		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2002BLO/PAU		262.5–318.9	27		0.40	99.55	melpt	sat	BDHT	1992KAB/KOZ
2002STE/CHI1		300.0–660.0	19	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1971HAL/BAL	suspect value

Correlated heat capacities (45.48.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1971HAL/BAL	297.1	1	3.00	#	0.002	1.66−3	0.01	−1.66−3	0
1996ROU/HER	298.1	1	0.50	#	1.074	1.41−1	0.54	1.41−1	1
2002BLO/PAU	262.5–318.9	27	0.40		0.347	3.58−2	0.14	−6.29−3	1
2002STE/CHI1	300.0–660.0	19	1.00		0.468	1.61−1	0.47	2.89−2	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1886SCH	(5.89−1, 2.10, 5.83−1, 6)	1979FUC	(5.44−1, 2.04, 5.44−1, 1)

Parameters of cubic spline polynomials (45.48.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	55	48	0.446	1.12−1	0.34	1.08−2	5
sat	55	48	0.428	9.72−2	0.31	1.10−2	3

T/K	A_1	A_2	A_3	A_4	Uncert.
262.5–530.0	3.131 57+1	−9.245 88	3.272 86	−2.554 40−1	II
530.0–660.0	−4.008 11+2	2.353 54+2	−4.287 81+1	2.647 13	III
262.5–530.0	3.136 45+1	−9.319 31	3.305 12	−2.598 16−1	II
530.0–660.0	−2.836 51+2	1.689 91+2	−3.033 84+1	1.856 12	III

Parameters of quasipolynomial equation (45.48.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	55	48	0.905	2.70−1	0.76	4.41−2	12

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
262.5–660.0	702.00	−2.431 09	4.798 79−2	1.707 16+1	1.517 05+1	6.239 13	8.182 90−1	IV

Deviation plot for 3–Methyl benzoate (45–048) is given in Fig. 118.

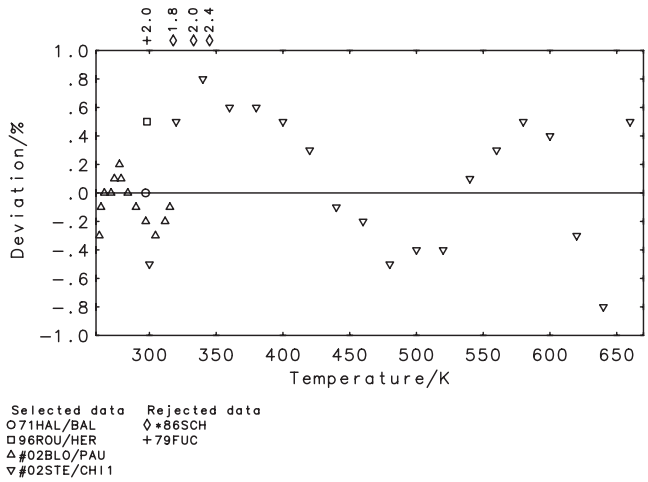

FIG. 118. Deviation plot for methyl benzoate (45-048).

6.5.5.7. Ethyl benzoate (45-064)

Name:	Ethyl benzoate
Formula:	$C_9H_{10}O_2$
CAS-RN:	93-89-0
Group No:	45-064

Experimental heat capacities (45.64.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1886SCH		318.4–345.6	5	S	n/a	n/a	n/a	avg	DSIO	1886SCH
1934KOL/UDO2	N	292.7	1		n/a	n/a	n/a	*p*	BSIT	1934KOL/UDO2
1936KUR/VOS	N	311.6	1		n/a	n/a	n/a	avg	DSIO	1936KUR/VOS
1979FUC		298.1	1		0.50	99.	chrom	*p*	BSIO	1980FUC
1996ROU/HER		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2002STE/CHI1		300.0–680.0	20	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1934KOL/UDO2	same datum in 1933KOL/UDO
1936KUR/VOS	average value in the temperature range 290–333 K

Correlated heat capacities (45.64.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1886SCH	318.4–345.6	5	3.00	#	0.580	5.53−1	1.74	5.36−1	5
1934KOL/UDO2	292.7	1	3.00	#	0.325	2.84−1	0.97	−2.84−1	−1
1979FUC	298.1	1	0.50		0.088	1.31−2	0.04	−1.31−2	−1
1996ROU/HER	298.1	1	0.50	#	0.415	6.15−2	0.21	6.15−2	1
2002STE/CHI1	300.0–680.0	20	1.00		0.505	2.31−1	0.50	−1.97−2	−3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1936KUR/VOS	(3.86, 11.35, 3.86, 1)

Parameters of cubic spline polynomials (45.64.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	29	28	0.554	3.41−1	0.96	7.33−2	1
sat	29	28	0.461	3.01−1	0.90	7.14−2	0

T/K	A_1	A_2	A_3	A_4	Uncert.
292.7–580.0	3.330 30+1	−8.497 42	3.137 99	−2.362 90−1	II
580.0–680.0	−1.522 01+3	7.959 77+2	−1.355 64+2	7.735 12	III
292.7–580.0	3.352 80+1	−8.778 27	3.242 43	−2.482 71−1	II
580.0–680.0	−9.226 87+2	4.858 16+2	−8.203 24+1	4.652 58	III

Parameters of quasipolynomial equation (45.64.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	29	28	0.838	3.24−1	0.87	1.59−2	3

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
292.7–680.0	707.00	−2.511 36	2.427 47−1	7.284 55	6.297 49+1	−3.857 62+1	8.554 97	III

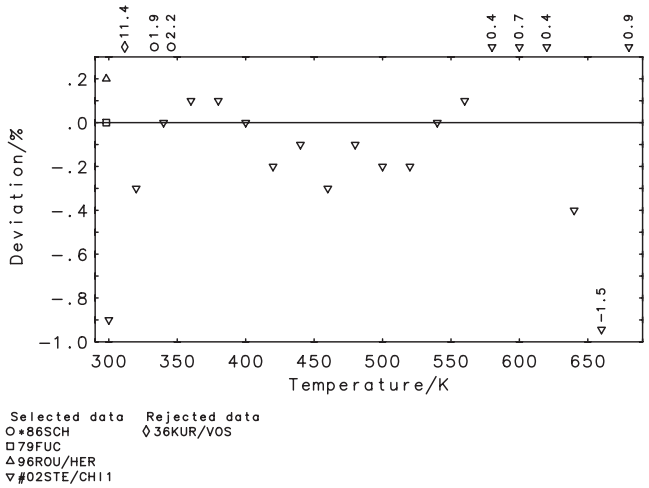

FIG. 119. Deviation plot for ethyl benzoate (45-064).

Deviation plot for Ethyl benzoate (45–064) is given in Fig. 119.

6.5.5.8. Methyl octanoate (45-070)

Name:	Methyl octanoate
Formula:	$C_9H_{18}O_2$
CAS-RN:	111-11-5
Group No:	45-070

Experimental heat capacities (45.70.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1988PIN/BRA		298.1	1		n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991DES/PAT		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2004VAN/OON		240.0–350.0	12	S	0.20	99.8	chrom	*p*	BSAO	1998VAN/VAN

Correlated heat capacities (45.70.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1988PIN/BRA	298.1	1	0.50	#	0.598	1.13−1	0.30	−1.13−1	−1
1991DES/PAT	298.1	1	0.50	#	0.204	3.86−2	0.10	3.86−2	1
2004VAN/OON	240.0–350.0	12	0.20		0.657	4.95−2	0.13	1.13−3	3

Parameters of regression polynomial (45.70.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	14	14	0.747	6.61−2	0.18	−4.34−3	3

T/K	A_1	A_2	A_3	A_4	Uncert.
240.0–350.0	1.000 42+2	−6.696 13+1	2.239 98+1	−2.324 60	III

Deviation plot for Methyl octanoate (45–070) is given in Fig. 120.

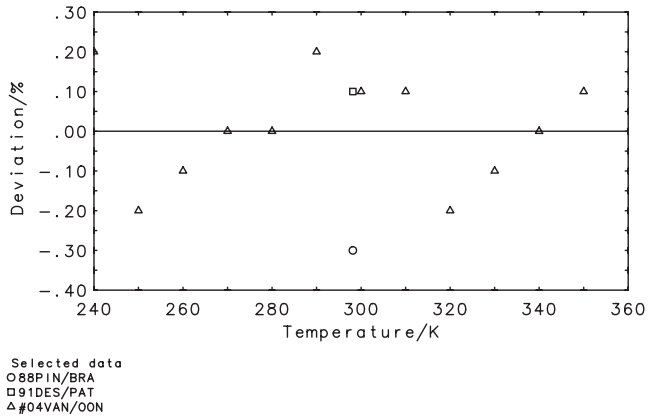

FIG. 120. Deviation plot for methyl octanoate (45-070).

6.5.5.9. Dimethyl 1,2-benzenedicarboxylate (45-076)

Name:	Dimethyl 1,2-benzenedicarboxylate
Formula:	$C_{10}H_{10}O_4$
CAS-RN:	131-11-3
Group No:	45-076

Experimental heat capacities (45.76.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1978MIL		274.0–370.0	eqn		1.00	99.	chrom	*p*	BDHT	1969PER/COM
1986RAB/NOV	N	274.2–360.0	11	S	0.50	n/a	n/a	*p*	BDAO	1951POP/GAL
1998ROH/MUS		308.0–447.2	31		1.00	99.95	chrom	*p*	BDCT	1991BAN/GAR
2002ROH/FUL	N	283.1–323.1	3		0.50	99.95	chrom	*p*	BDCT	1991BAN/GAR

Reference	Notes
1986RAB/NOV	some data in 1969RAB/MAR and 1970MAR/RAB; adiabatic calorimeter used in 1956POP/KOL below 300 K
2002ROH/FUL	same data in 2000ROH (thesis) and 1999ROH/MUS

6.5.5.10. Octyl acetate (45-085)

Name:	Octyl acetate
Formula:	$C_{10}H_{20}O_2$
CAS-RN:	112-14-1
Group No:	45-085

Experimental heat capacities (45.85.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991DES/PAT		298.1	1	n/a	98.	anal	*p*	FSIT	1971PIC/LED
1997SVO/GOT		300.3–318.8	5	0.30	99.9	chrom	*p*	BSAO	1991SVO/ZAB1
2001BEC/GME		310.0–420.0	23	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

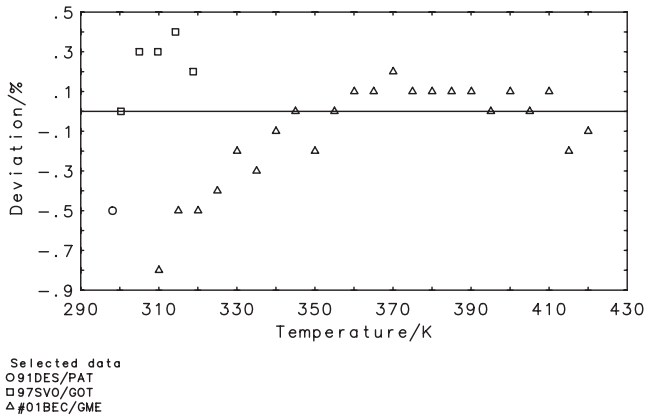

FIG. 121. Deviation plot for octyl acetate (45-085).

Correlated heat capacities (45.85.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1991DES/PAT	298.1	1	0.50	#	0.913	1.89−1	0.46	−1.89−1	−1
1997SVO/GOT	300.3–318.8	5	0.30		0.842	1.07−1	0.25	9.44−2	4
2001BEC/GME	310.0–420.0	23	0.50		0.555	1.19−1	0.28	−4.77−2	−3

Parameters of regression polynomial (45.85.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	29	29	0.664	1.27−1	0.30	−2.81−2	0	
T/K		A_1		A_2	A_3		A_4	Uncert.
298.1–420.0		3.937 19+1		−3.479 49	1.409 93			II

Deviation plot for Octyl acetate (45–085) is given in Fig. 121.

6.5.5.11. Methyl decanoate (45-089)

Name:	Methyl decanoate
Formula:	$C_{11}H_{22}O_2$
CAS-RN:	110-42-9
Group No:	45-089

Experimental heat capacities (45.89.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1979FUC		298.1	1		0.50	99.	chrom	p	BSIO	1980FUC
2004VAN/OON		270.0–350.0	9	S	0.20	99.8	chrom	p	BSAO	1998VAN/VAN

Correlated heat capacities (45.89.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004VAN/OON	270.0–350.0	9	0.20	0.785	7.03−2	0.16	1.83−4	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1979FUC	(8.31−1, 1.80, 8.31−1, 1)

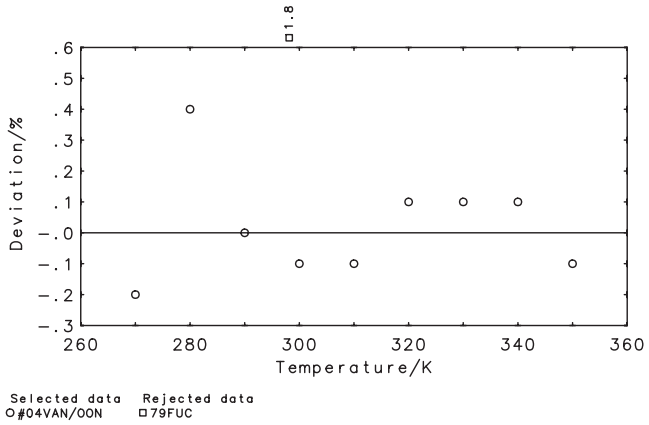

FIG. 122. Deviation plot for methyl decanoate (45-089).

Parameters of regression polynomial (45.89.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	9	1.053	9.43−2	0.21	1.83−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
270.0–350.0	−1.334 96+2	1.643 37+2	5.164 69+1	5.578 20	IV

Deviation plot for Methylbutyl decanoate (45–089) is given in Fig. 122.

6.5.5.12. Diethyl 1,2-benzenedicarboxylate (45-090)

Name:	Diethyl 1,2-benzenedicarboxylate
Formula:	$C_{12}H_{14}O_4$
CAS-RN:	84-66-2
Group No:	45-090

Experimental heat capacities (45.90.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1967CHA/HOR		273.0–353.4	25	0.10	99.88	melpt	p	BSAO	1965STE/BLA
1979FUC		298.1	1	0.50	99.	chrom	p	BSIO	1980FUC
2000ROH		313.1–372.7	18	1.00	99.93	chrom	p	BDCT	1991BAN/GAR
2001BEC/GME		311.3–415.0	22	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF
2002ROH/FUL	N	283.1–323.1	3	0.50	99.93	chrom	p	BDCT	1991BAN/GAR

Reference	Notes
2002ROH/FUL	same data in 2000ROH (thesis) and 1998ROH/SCH

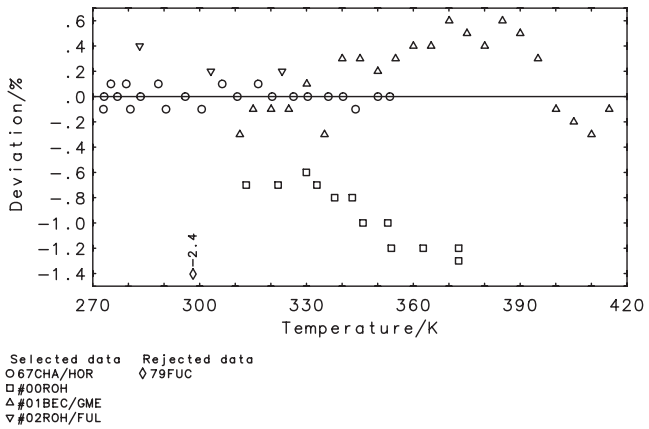

FIG. 123. Deviation plot for diethyl 1,2-benzenedicarboxylate (45-090).

Correlated heat capacities (45.90.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1967CHA/HOR	273.0–353.4	25	0.10	0.649	2.85−2	0.06	1.50−5	−2
2000ROH	313.1–372.7	18	1.00	0.921	4.31−1	0.92	−4.14−1	−18
2001BEC/GME	311.3–415.0	22	0.50	0.660	1.61−1	0.33	7.32−2	4
2002ROH/FUL	283.1–323.1	3	0.50	0.518	1.14−1	0.26	1.09−1	3

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1979FUC	(1.02, 2.37, −1.02, −1)

Parameters of regression polynomial (45.90.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	69	68	0.746	2.47−1	0.53	−8.10−2	−13

T/K	A_1	A_2	A_3	A_4	Uncert.
273.0–415.0	3.463 50+1	5.924 02−1	8.593 20−1		III

Parameters of quasipolynomial equation (45.90.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	69	68	1.265	2.29−1	0.48	−2.29−3	4

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
273.0–415.0	760.20	1.011 40+2	3.325 78+1	−4.066 46	1.094 10+2	−6.397 45	2.974 35+1	V

Deviation plot for Diethyl 1,2–benzenedicarboxylate (45–090) is given in Fig. 123.

6.5.5.13. Methyl tetradecanoate (45-103)

Name:	Methyl tetradecanoate
Formula:	$C_{15}H_{30}O_2$
CAS-RN:	124-10-7
Group No:	45-103

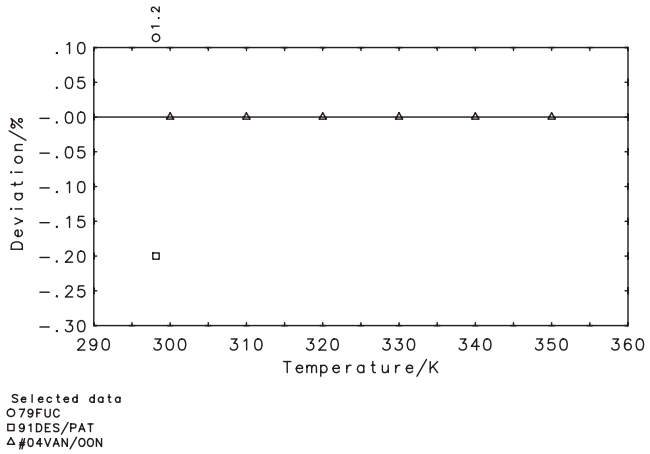

FIG. 124. Deviation plot for methyl tetradecanoate (45-103).

Experimental heat capacities (45.103.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		292.1	1		n/a	n/a	n/a	*p*	DSIO	1924GAR/RAN
1979FUC		298.1	1		0.50	99.	chrom	*p*	BSIO	1980FUC
1991DES/PAT		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2004VAN/OON		300.0–350.0	6	S	0.20	99.5	chrom	*p*	BSAO	1998VAN/VAN

Correlated heat capacities (45.103.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979FUC	298.1	1	1.00	#	1.247	7.58−1	1.25	7.58−1	1
1991DES/PAT	298.1	1	0.50	#	0.476	1.43−1	0.24	−1.43−1	−1
2004VAN/OON	300.0–350.0	6	0.20		0.150	1.87−2	0.03	−1.09−3	0

Parameters of regression polynomial (45.103.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	9	8	0.619	3.46−1	0.57	7.61−2	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–350.0	6.384 21+1	−8.121 29	2.294 76		III

Deviation plot for Methyl tetradecanoate (45–103) is given in Fig. 124.

6.5.5.14. Dibutyl 1,2-benzenedicarboxylate (45-104)

Name:	Dibutyl 1,2-benzenedicarboxylate
Formula:	$C_{16}H_{22}O_4$
CAS-RN:	84-74-2
Group No:	45-104

Experimental heat capacities (45.104.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1948BER/MEL		353.1–423.1	2		n/a	n/a	n/a	*p*	BSIO	1934LON/REY
1970MAR/RAB	N	173.5–360.0	5	S	0.30	n/a	n/a	*p*	BSAO	1956POP/KOL
1985RAB/NOV		173.9–300.1	40		n/a	99.7	chrom	*p*	BSAO	1966NIK/LEB

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002ROH/FUL	N	312.8–447.3	30	1.00	99.97	chrom	p	BDCT	1991BAN/GAR

Reference	Notes
1970MAR/RAB	same data in 1969RAB/MAR at 300 and 360 K
2002ROH/FUL	same data in 2000ROH (thesis)

Correlated heat capacities (45.104.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1970MAR/RAB	200.0–360.0	4	0.30		2.894	5.35−1	0.87	−2.13−1	2
1985RAB/NOV	201.6–300.1	29	0.50	#	0.513	1.37−1	0.26	−2.35−2	−3
2002ROH/FUL	312.8–447.3	30	1.00		0.355	2.29−1	0.35	−4.77−3	−6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1948BER/MEL	(2.37, 3.31, 1.76, 2)

Parameters of cubic spline polynomials (45.104.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	77	75	1.604	3.70−1	0.78	7.79−2	26

T/K	A_1	A_2	A_3	A_4	Uncert.
173.5–180.0	−2.480 38+5	4.134 95+5	−2.297 27+5	4.254 32+4	IV
180.0–320.0	8.350 67+1	−4.081 78+1	1.567 36+1	−1.656 82	III
320.0–447.3	1.262 41+1	2.563 46+1	−5.092 81	5.063 43−1	IV

Parameters of quasipolynomial equation (45.104.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	77	63	0.873	2.35−1	0.38	−2.66−2	−7

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
200.0–447.3	790.00	4.349 41+3	5.493 99+2	−5.008 63+2	3.835 80+3	1.314 90+3	1.891 23+3	IV

Deviation plot for Dibutyl 1,2–benzenedicarboxylate (45–104) is given in Fig. 125.

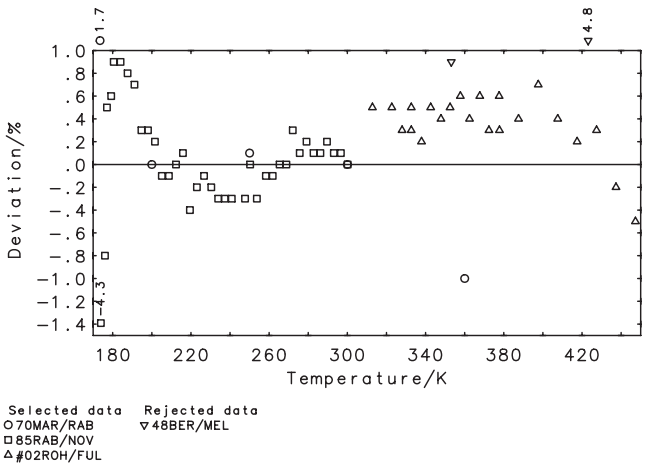

FIG. 125. Deviation plot for dibutyl 1,2-benzenedicarboxylate (45-104).

6.5.5.15. Bis(2-ethylhexyl)-1,2-benzenedicarboxylate (45-110)

Name:	Bis(2-ethylhexyl)-1,2-benzenedicarboxylate
Formula:	$C_{24}H_{38}O_4$
CAS-RN:	117-81-7
Group No:	45-110

Experimental heat capacities (45.110.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1970MAR/RAB	N	182.5–360.0	5	S	0.30	n/a	n/a	p	BSAO	1956POP/KOL
1985RAB/NOV		184.4–300.2	38		n/a	99.7	chrom	p	BSAO	1966NIK/LEB
2002ROH/FUL	N	313.0–461.9	35		1.00	99.64	chrom	p	BDCT	1991BAN/GAR

Reference	Notes
1970MAR/RAB	same data in 1969RAB/MAR at/300 and 360 K
2002ROH/FUL	same data in 2000ROH (thesis)

Correlated heat capacities (45.110.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1970MAR/RAB	200.0–360.0	4	0.30		2.336	6.42−1	0.70	−2.47−1	0
1985RAB/NOV	200.0–300.2	32	0.50	#	0.314	1.25−1	0.16	−3.96−2	−18
2002ROH/FUL	313.0–461.9	35	1.00		0.337	3.33−1	0.34	3.34−2	1

Parameters of cubic spline polynomials (45.110.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	78	78	0.837	3.40−1	0.43	1.03−1	15

T/K	A_1	A_2	A_3	A_4	Uncert.
182.5–195.0	−6.483 69+4	9.988 20+4	−5.122 98+4	8.758 71+3	III
195.0–370.0	1.213 26+2	−5.374 24+1	1.933 42+1	−1.825 08	III
370.0–461.9	−1.236 66+1	5.465 70+1	−9.962 96	8.142 95−1	IV

Parameters of quasi-polynomial equation (45.110.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	78	71	0.658	3.00−1	0.32	−1.53−2	−17

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
200.0–461.9	784.00	6.519 30+3	7.933 20+2	−7.225 93+2	5.819 50+3	1.798 41+3	3.151 53+3	III

Deviation plot for Bis(2–ethylhexyl)—1,2–benzenedicarboxylate (45–110) is given in Fig. 126.

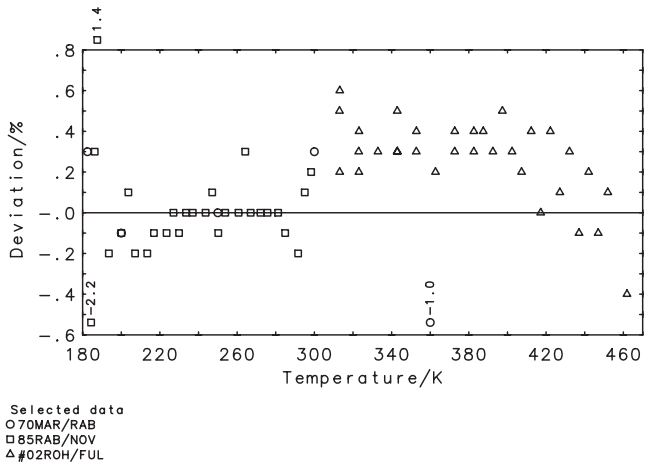

FIG. 126. Deviation plot for bis(2-ethylhexyl)-1,2-benzenedicarboxylate (45-110).

6.5.5.16. 1,2,3-Propanetriyl ester dodecanoic acid (45-120)

Name:	1,2,3-Propanetriyl ester dodecanoic acid
Formula:	$C_{39}H_{74}O_6$
CAS-RN:	538-24-9
Group No.:	45-120

Experimental heat capacities (45.120.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1947CHA/SIN		330.9–370.2	6	n/a	98.	estim	*p*	BSAO	1944BAI/TOD
1976PHI/MAT	N	323.0–398.0	4	n/a	n/a	n/a	*p*	BDHT	1973PER/COM
1995MOR/IDR1		328.0–443.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		328.0–443.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		443.0–523.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
2000MOR/KAM		353.1–453.1	6	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1

Reference	Notes
1976PHI/MAT	reproducibility given as 5%

Correlated heat capacities (45.120.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1995MOR/IDR1	328.0–443.5	16	2.00	#	0.048	1.60−1	0.10	2.34−3	−2
1995MOR/IDR2	328.0–443.5	16	2.00	#	0.048	1.61−1	0.10	1.48−2	−2
1995MOR/IDR2	443.0–522.8	8	2.00	#	0.066	2.44−1	0.13	−1.35−1	−4
2000MOR/KAM	353.1–453.1	6	1.00		0.125	2.21−1	0.12	3.49−2	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1947CHA/SIN	(5.93, 3.57, 5.92, 6)	1976PHI/MAT	(2.86, 1.82, −2.41, −3)

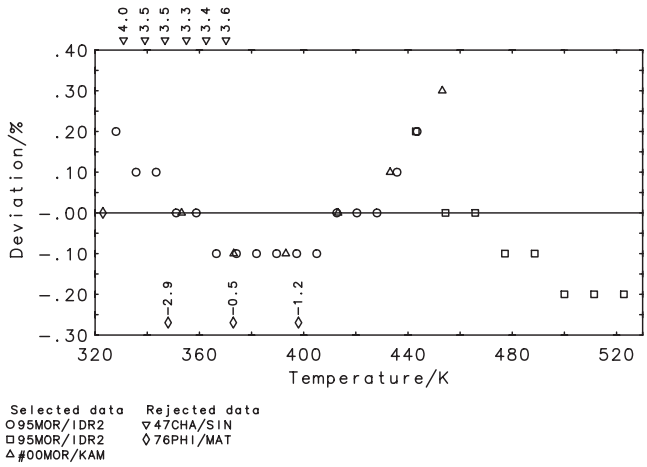

FIG. 127. Deviation plot for 1,2,3-propanetriyl ester dodecanoic acid (45-120).

Parameters of regression polynomial (45.120.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	56	46	0.069	1.93−1	0.11	−1.30−2	−10	
T/K		A_1		A_2		A_3	A_4	Uncert.
328.0–522.8		7.353 89+1		2.980 80+1		−1.428 75		III

Deviation plot for 1,2,3–Propanetriyl ester dodecanoic acid (45–120) is given in Fig. 127.

6.5.5.17. 1,2,3-Propanetriyl ester tetradecanoic acid (45-124)

Name:	1,2,3-Propanetriyl ester tetradecanoic acid
Formula:	$C_{45}H_{86}O_6$
CAS-RN:	555-45-3
Group No:	45-124

Experimental heat capacities (45.124.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1947CHA/SIN		331.5–365.0	6	n/a	98.	estim	*p*	BSAO	1944BAI/TOD
1976PHI/MAT	N	333.0–433.0	5	n/a	n/a	n/a	*p*	BDHT	1973PER/COM
1995MOR/IDR2		338.0–454.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		454.0–523.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
2000MOR/KAM		353.1–453.1	6	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1

Reference	Notes
1976PHI/MAT	reproducibility given as 5%

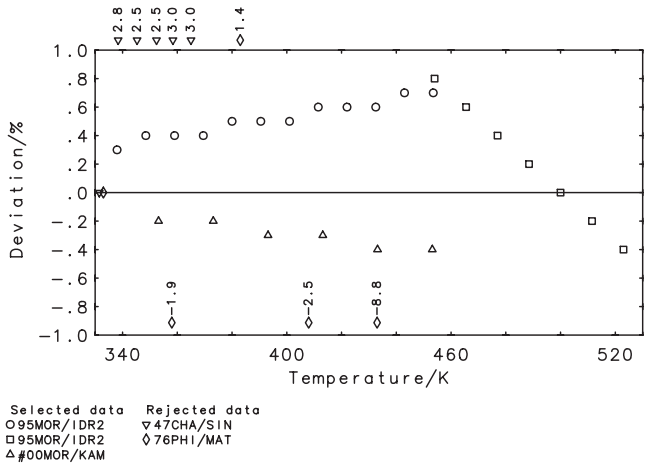

FIG. 128. Deviation plot for 1,2,3-propanetriyl ester tetradecanoic acid (45-124).

Correlated heat capacities (45.124.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1995MOR/IDR2	338.0–453.5	12	2.00	#	0.266	1.06	0.53	1.02	12
1995MOR/IDR2	454.0–523.0	7	2.00	#	0.220	9.27−1	0.44	4.40−1	3
2000MOR/KAM	353.1–453.1	6	1.00		0.329	6.55−1	0.33	−6.27−1	−6

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1947CHA/SIN	(5.29, 2.76, 5.27, 5)	1976PHI/MAT	(8.82, 4.74, −5.50, −2)

Parameters of regression polynomial (45.124.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	36	25	0.289	1.00	0.50	4.63−1	9	
T/K		A_1		A_2	A_3	A_4		Uncert.
338.0–523.0		1.164 60+2		1.948 41+1	6.754 27−2			IV

Deviation plot for 1,2,3–Propanetriyl ester tetradecanoic acid (45–124) is given in Fig. 128.

6.5.5.18. 1,2,3-Propanetriyl ester hexadecanoic acid (45-127)

Name:	1,2,3-Propanetriyl ester hexadecanoic acid
Formula:	$C_{51}H_{98}O_6$
CAS-RN:	555-44-2
Group No:	45-127

Experimental heat capacities (45.127.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1947CHA/SIN		338.8–369.1	6	n/a	98.	estim	p	BSAO	1944BAI/TOD
1976PHI/MAT	N	343.0–418.0	4	n/a	n/a	n/a	p	BDHT	1973PER/COM
1982OLL/PER		340.0	1	n/a	n/a	n/a	p	BDHT	1973PER/COM
1993KAP/BAL		345.0–365.0	2	n/a	99.	anal	p	BDCT	1986MER/BEN
1995MOR/IDR2		348.0–457.0	eqn	n/a	99.0	anal	p	BDHT	1995MOR/IDR1
1995MOR/IDR2		457.0–523.0	eqn	n/a	99.0	anal	p	BDHT	1995MOR/IDR1
1999VAN/TEN		341.2–354.9	7	0.20	96.9	melpt	p	BSAO	1998VAN/VAN

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000MOR/KAM		353.1–453.1	6	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1

Reference	Notes
1976PHI/MAT	reproducibility given as 5%

6.5.5.19. 1,2,3-Propanetriyl ester octadecanoic acid (45-130)

Name:	1,2,3-Propanetriyl ester octadecanoic acid
Formula:	$C_{57}H_{110}O_6$
CAS-RN:	555-43-1
Group No:	45-130

Experimental heat capacities (45.130.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1947CHA/SIN		346.5–371.6	6	n/a	98.	estim	*p*	BSAO	1944BAI/TOD
1976PHI/MAT	N	353.0–453.0	5	n/a	n/a	n/a	*p*	BDHT	1973PER/COM
1995MOR/IDR2		353.0–460.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		460.0–523.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
2000MOR/KAM	N	353.1–453.1	6	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1
2005MAT/VAN		349.1–369.7	10	0.50	99.0	anal	*p*	BSAO	2002VAN/VAN1
2005MAT/VAN	N	346.8–370.0	11	1.00	99.0	anal	*p*	BSAO	2002VAN/VAN1

Reference	Notes
1976PHI/MAT	reproducibility given as 5 %
2000MOR/KAM	wrong published data corrected based on the response from the author
2005MAT/VAN	β-phase

6.5.5.20. Dimethyl ester propanedioic acid (45-132)

Name:	Dimethyl ester propanedioic acid
Formula:	$C_5H_8O_4$
CAS-RN:	108-59-8
Group No:	45-132

Experimental heat capacities (45.132.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1992VER/BEC		298.1	1		n/a	99.995	chrom	*p*	BDHT	1969PER/COM
2002STE/CHI5		300.0–620.0	16	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (45.132.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002STE/CHI5	300.0–620.0	16	1.00	0.918	2.26−1	0.92	4.94−3	0

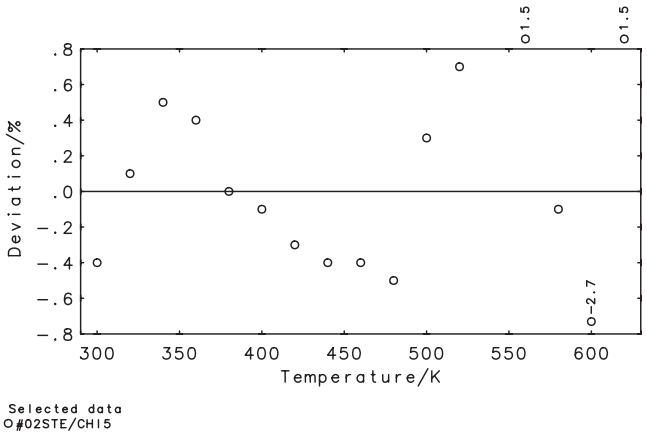

FIG. 129. Deviation plot for dimethyl ester propanedioic acid (45-132).

Parameters of cubic spline polynomials (45.132.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	17	16	1.107	2.72−1	1.11	4.94−3	0
sat	17	16	0.811	1.86−1	0.81	2.32−3	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
300.0–520.0	4.680 05+1	−2.378 72+1	6.251 02	−5.007 40−1	II
520.0–620.0	−1.130 35+3	6.553 37+2	−1.243 50+2	7.871 10	IV
300.0–520.0	4.500 02+1	−2.254 22+1	5.981 76	−4.831 36−1	II
520.0–620.0	−7.282 65+2	4.235 72+2	−7.980 95+1	5.016 31	IV

Parameters of quasi-polynomial equation (45.132.4)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	17	16	1.081	2.31−1	1.08	4.23−3	0

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
300.0–620.0	647.00	2.082 32	4.629 93−1	3.655 26	4.976 16+1	−4.873 86+1	2.021 85+1	IV

Deviation plot for Dimethyl ester propanedioic acid (45–132) is given in Fig. 129.

6.5.5.21. Butyl phenylmethyl ester 1,2-benzenedicarboxylic acid (45-149)

Name:	Butyl phenylmethyl ester 1,2-benzenedicarboxylic acid
Formula:	$C_{19}H_{20}O_4$
CAS-RN:	85-68-7
Group No:	45-149

Experimental heat capacities (45.149.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002ROH/FUL	N	313.1–382.7	20	1.00	99.82	chrom	*p*	BDCT	1991BAN/GAR

Reference	Notes
2002ROH/FUL	same data in 2000ROH (thesis)

6.5.5.22. 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester hexadecanoic acid (45-155)

Name: 2,3-Bis[(1-oxotetradecyl)oxy]propyl ester hexadecanoic acid

Formula: $C_{47}H_{90}O_6$
CAS-RN: 60138-13-8
Group No: 45-155

Experimental heat capacities (45.155.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1995MOR/IDR2		333.0–454.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		454.0–523.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
2000MOR/KAM		353.1–453.1	6	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1

6.5.5.23. 1-[[(1-Oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (*Z*)-9-octadecenoic acid (45-158)

Name: 1-[[(1-Oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (*Z*)-9-octadecenoic acid

Formula: $C_{55}H_{102}O_6$
CAS-RN: 2190-30-9
Group No: 45-158

Experimental heat capacities (45.158.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1995MOR/IDR2		308.0–435.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
1995MOR/IDR2		435.0–523.0	eqn	n/a	99.0	anal	*p*	BDHT	1995MOR/IDR1
2000MOR/KAM		333.1–453.1	7	1.00	n/a	n/a	*p*	BDHT	1995MOR/IDR1

6.5.5.24. Ethyl methyl carbonate (45-161)

Name: Ethyl methyl carbonate

Formula: $C_4H_8O_3$
CAS-RN: 623-53-0
Group No: 45-161

Experimental heat capacities (45.161.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004DIN		220.0–323.0	eqn	n/a	n/a	n/a	*p*	BDHT	1998SAL/FER

Parameters of regression polynomial (45.161.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	12	12	0.000	9.42−9	0.00	−2.48−9	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
220.0–323.4		1.316 14−1		2.651 28−2				V

6.5.5.25. Cyclohexyl formate (45-162)

Name:	Cyclohexyl formate
Formula:	$C_7H_{12}O_2$
CAS-RN:	4351-54-6
Group No:	45-162

Experimental heat capacities (45.162.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001KOZ/BLO	N	206.5–309.4	26	S	0.40	99.51	melpt	sat	BSAO	1993DIK/KAB

Reference	Notes
2001KOZ/BLO	smoothed values in 2004PAU/ZAI

Parameters of regression polynomial (45.162.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	26	26	0.403	4.00−2	0.16	1.09−4	5

T/K	A_1	A_2	A_3	A_4	Uncert.
206.5–309.4	2.542 21+1	−3.905 96	1.419 12		II

6.5.5.26. Cyclohexyl acetate (45-163)

Name:	Cyclohexyl acetate
Formula:	$C_8H_{14}O_2$
CAS-RN:	622-45-7
Group No:	45-163

Experimental heat capacities (45.163.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1992SIM/KOZ		224.4–298.1	3	S	0.40	99.85	chrom	sat	BSAO	1993DIK/KAB
2001KOZ/BLO	N	225.2–311.0	13	S	0.40	99.85	chrom	sat	BSAO	1993DIK/KAB

Reference	Notes
2001KOZ/BLO	smoothed values and same data in 2004PAU/ZAI; eq. $C_p=f(T)$ in 2004ZAI/PAV

Correlated heat capacities (45.163.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1992SIM/KOZ	224.4–298.1	3	0.40	0.170	1.82−2	0.07	6.63−3	1
2001KOZ/BLO	225.2–311.0	13	0.40	0.171	1.87−2	0.07	−1.50−3	1

Parameters of regression polynomial (45.163.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	16	16	0.190	2.07−2	0.08	2.54−5	2

T/K	A_1	A_2	A_3	A_4	Uncert.
224.4–311.0	2.306 52+1	−4.166 71−1	8.659 82−1		II

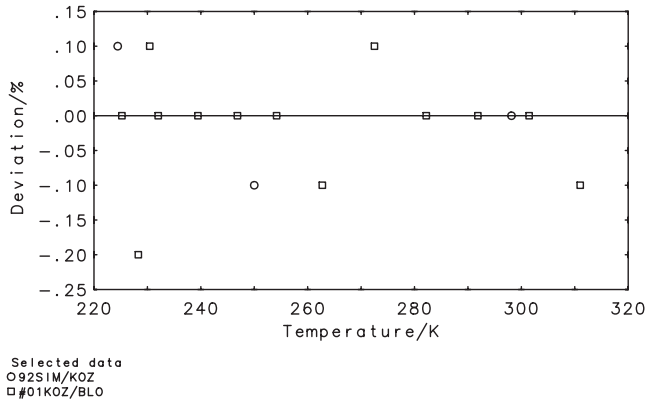

FIG. 130. Deviation plot for cyclohexyl acetate (45-163).

Deviation plot for Cyclohexyl acetate (45–163) is given in Fig. 130.

6.5.5.27. Methyl-2-methylbenzoate (45-164)

Name:	Methyl-2-methylbenzoate
Formula:	$C_9H_{10}O_2$
CAS-RN:	89-71-4
Group No:	45-164

Experimental heat capacities (45.164.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002BLO/PAU		230.1–300.4	17	0.40	99.8	melpt	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (45.164.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−			
sat	17	17	0.170	1.94−2	0.07	2.41−5	−3			
T/K			A_1		A_2		A_3		A_4	Uncert.
230.1–300.4			9.328 34+1		−7.728 52+1		2.938 30+1		−3.580 41	II

6.5.5.28. Methyl ester 3-methylbenzoic acid (45-165)

Name:	Methyl ester 3-methylbenzoic acid
Formula:	$C_9H_{10}O_2$
CAS-RN:	99-36-5
Group No:	45-165

Experimental heat capacities (45.165.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002BLO/PAU		271.6–310.4	9	0.40	99.42	melpt	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (45.165.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	9	9	0.277	3.28−2	0.11	6.04−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
271.6–310.4	1.522 56+1	4.929 29			II

6.5.5.29. Methyl ester 4-methylbenzoic acid (45-166)

Name:	Methyl ester 4-methylbenzoic acid
Formula:	$C_9H_{10}O_2$
CAS-RN:	99-75-2
Group No:	45-166

Experimental heat capacities (45.166.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002BLO/PAU		308.9–321.7	8	0.40	99.71	Melpt	sat	BDHT	1992KAB/KOZ

Parameters of regression polynomial (45.166.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	8	8	0.179	2.14−2	0.07	2.46−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
308.9–321.7	1.373 75+1	5.179 97			II

6.5.5.30. Cyclohexyl ester propanoic acid (45-167)

Name:	Cyclohexyl ester propanoic acid
Formula:	$C_9H_{16}O_2$
CAS-RN:	6222-35-1
Group No:	45-167

Experimental heat capacities (45.167.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004PAU/ZAI		298.1–340.0	6	S	0.40	99.7	chrom	p	BSAO	1993DIK/KAB

Parameters of regression polynomial (45.167.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	0.029	3.84−3	0.01	6.36−7	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–340.0	2.055 18+1	4.232 22			II

6.5.5.31. (2*E*)-Methyl ester 3-phenyl-2-propenoic acid (45-168)

Name:	(2*E*)-Methyl ester 3-phenyl-2-propenoic acid
Formula:	$C_{10}H_{10}O_2$
CAS-RN:	1754-62-7
Group No:	45-168

Experimental heat capacities (45.168.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI4		309.0–550.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (45.168.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	15	15	0.000	1.83−6	0.00	−2.54−7	0
T/K		A_1		A_2	A_3	A_4	Uncert.
309.0–549.8		1.680 00+1		5.300 00			III

6.5.5.32. Cyclohexyl ester butanoic acid (45-169)

Name:	Cyclohexyl ester butanoic acid
Formula:	$C_{10}H_{18}O_2$
CAS-RN:	1551-44-6
Group No:	45-169

Experimental heat capacities (45.169.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001KOZ/BLO	N	221.6–307.1	26	S	0.40	98.43	melpt	sat	BSAO	1993DIK/KAB
Reference	Notes									
2001KOZ/BLO	smoothed values in 2004PAU/ZAI									

Parameters of regression polynomial (45.169.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
sat	26	26	0.148	2.01−2	0.06	2.33−5	−2		
T/K		A_1		A_2		A_3		A_4	Uncert.
221.6–307.1		1.278 60+2		−1.135 60+2		4.356 24+1		−5.295 49	II

6.5.5.33. Methyl nonanoate (45-170)

Name:	Methyl nonanoate
Formula:	$C_{10}H_{20}O_2$
CAS-RN:	1731-84-6
Group No:	45-170

Experimental heat capacities (45.170.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		240.0–350.0	12	S	0.20	99.7	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.170.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.575	4.71−2	0.12	6.83−5	3

T/K	A_1	A_2	A_3	A_4	Uncert.
240.0–350.0	9.306 93+1	−5.611 59+1	1.864 73+1	−1.885 14	II

6.5.5.34. Cyclohexyl ester pentanoic acid (45-171)

Name:	Cyclohexyl ester pentanoic acid
Formula:	$C_{11}H_{20}O_2$
CAS-RN:	1551-43-5
Group No:	45-171

Experimental heat capacities (45.171.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001KOZ/BLO	N	223.8–311.0	23	S	0.40	99.17	melpt	sat	BSAO	1993DIK/KAB

Reference	Notes
2001KOZ/BLO	smoothed values in 2004PAU/ZAI

Parameters of regression polynomial (45.171.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	23	23	0.264	3.93−2	0.11	6.98−5	2

T/K	A_1	A_2	A_3	A_4	Uncert.
223.8–311.0	3.762 10+1	−5.092 82	1.845 72		II

6.5.5.35. Methyl undecanoate (45-172)

Name:	Methyl undecanoate
Formula:	$C_{12}H_{24}O_2$
CAS-RN:	1731-86-8
Group No:	45-172

Experimental heat capacities (45.172.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		270.0–350.0	9	S	0.20	99.5	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.172.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	9	9	0.431	4.35−2	0.09	4.58−5	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
270.0–350.0	4.901 39+1	−5.151 81	1.711 39		II

6.5.5.36. Ethyl undecanoate (45-173)

Name:	Ethyl undecanoate
Formula:	$C_{13}H_{26}O_2$
CAS-RN:	627-90-7
Group No:	45-173

Experimental heat capacities (45.173.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005VAN/OON	N	261.3–365.4	85	0.50	97.5	melpt	p	BSAO	2002VAN/VAN1

Parameters of regression polynomial (45.173.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	85	85	0.359	9.27−2	0.18	3.12−4	2	
T/K		A_1		A_2		A_3	A_4	Uncert.
261.3–365.4		5.891 47+1		−1.047 50+1		2.742 48		II

6.18.5.37. Methyl dodecanoate (45-174)

Name:	Methyl dodecanoate
Formula:	$C_{13}H_{26}O_2$
CAS-RN:	111-82-0
Group No:	45-174

Experimental heat capacities (45.174.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		280.0–350.0	8	S	0.20	99.5	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.174.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	8	8	0.445	4.67−2	0.09	4.77−5	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
280.0–350.0		−1.532 51+2		1.910 83+2		−6.070 06+1	6.630 90	III

6.5.5.38. Methyl tridecanoate (45-175)

Name:	Methyl tridecanoate
Formula:	$C_{14}H_{28}O_2$
CAS-RN:	1731-88-0
Group No:	45-175

Experimental heat capacities (45.175.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		290.0–340.0	6	S	0.20	99.8	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.175.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	0.243	2.76−2	0.05	1.53−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
290.0–340.0	6.101 91+1	−8.992 34	2.481 96		II

6.5.5.39. Ethyl tridecanoate (45-176)

Name:	Ethyl tridecanoate
Formula:	$C_{15}H_{30}O_2$
CAS-RN:	28267-29-0
Group No:	45-176

Experimental heat capacities (45.176.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005VAN/OON	N	274.8-320.1	23	0.20	99.3	melpt	p	BSAO	2002VAN/VAN1

Reference	Notes
2005VAN/OON	cal. 393, 1987VAN/VAN

Parameters of regression polynomial (45.176.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	23	22	0.282	3.34−2	0.06	3.47−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
275.3–320.1	9.940 08+1	−3.304 14+1	6.603 00		II

6.5.5.40. Methyl pentadecanoate (45-177)

Name:	Methyl pentadecanoate
Formula:	$C_{16}H_{32}O_2$
CAS-RN:	7132-64-1
Group No:	45-177

Experimental heat capacities (45.177.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		300.0–340.0	5	S	0.20	99.6	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.177.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.514	6.67−2	0.10	2.36−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
300.0–340.0	−1.813 09+3	1.731 08+3	−5.335 60+2	5.499 93+1	III

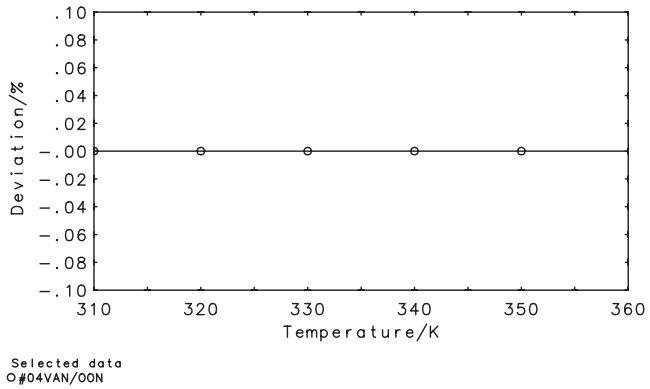

FIG. 131. Deviation plot for methyl hexadecanoate (45-178).

6.5.5.41. Methyl hexadecanoate (45-178)

Name:	Methyl hexadecanoate
Formula:	$C_{17}H_{34}O_2$
CAS-RN:	112-39-0
Group No:	45-178

Experimental heat capacities (45.178.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		303.1	1		n/a	n/a	n/a	p	DSIO	1924GAR/RAN
2004VAN/OON		310.0–350.0	5	S	0.20	99.3	chrom	p	BSAO	1998VAN/VAN

Correlated heat capacities (45.178.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004VAN/OON	310.0–350.0	5	0.20	0.028	3.98−3	0.01	−1.53−6	0

Parameters of regression polynomial (45.178.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	6	5	0.045	6.29−3	0.01	−1.53−6	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
310.0–350.0		7.850 69+1		−1.324 70+1		3.244 29		I

Deviation plot for Methyl hexadecanoate (45–178) is given in Fig. 131.

6.5.5.42. Methyl heptadecanoate (45-179)

Name:	Methyl heptadecanoate
Formula:	$C_{18}H_{36}O_2$
CAS-RN:	1731-92-6
Group No:	45-179

Experimental heat capacities (45.179.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004VAN/OON		310.0–350.0	5	S	0.20	99.0	chrom	p	BSAO	1998VAN/VAN

Parameters of regression polynomial (45.179.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.576	8.46−2	0.12	−1.56−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
310.0–350.0	−1.252 07+3	1.206 81+3	−3.679 75+2	3.757 05+1	III

6.5.5.43. Ethyl heptadecanoate (45-180)

Name:	Ethyl heptadecanoate
Formula:	$C_{19}H_{38}O_2$
CAS-RN:	14010-23-2
Group No:	45-180

Experimental heat capacities (45.180.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		301.15	2.09	n/a	n/a	n/a	p	DSIO	1924GAR/RAN

6.5.5.44. Methyl octadecanoate (45-181)

Name:	Methyl octadecanoate
Formula:	$C_{19}H_{38}O_2$
CAS-RN:	112-61-8
Group No:	45-181

Experimental heat capacities (45.181.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		311.1	1		n/a	n/a	n/a	p	DSIO	1924GAR/RAN
2004VAN/OON		320.0–350.0	4	S	0.20	99.0	chrom	p	BSAO	1998VAN/VAN

Correlated heat capacities (45.181.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936KIN/GAR	311.1	1	3.00	#	0.213	4.89−1	0.64	4.89−1	1
2004VAN/OON	320.0–350.0	4	0.20		0.094	1.47−2	0.02	−5.40−4	−1

Parameters of regression polynomial (45.181.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.200	3.47−1	0.45	9.74−2	0

T/K	A_1	A_2	A_3	A_4	Uncert.
311.1–350.0	9.654 53+1	−2.098 52+1	4.634 73		II

Deviation plot for Methyl octadecanoate (45–181) is given in Fig. 132.

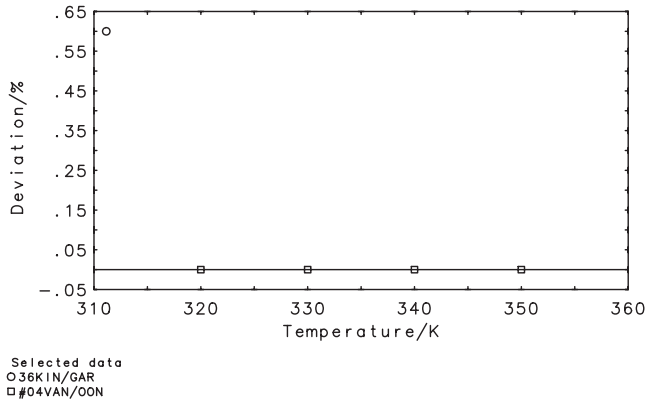

FIG. 132. Deviation plot for methyl octadecanoate (45-181).

6.5.5.45. Methyl nonadecanoate (45-182)

Name:	Methyl nonadecanoate
Formula:	$C_{20}H_{40}O_2$
CAS-RN:	1731-94-8
Group No:	45-182

Experimental heat capacities (45.182.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		312.1	1		n/a	n/a	n/a	*p*	DSIO	1924GAR/RAN
2004VAN/OON		320.0–350.0	4	S	0.20	99.7	chrom	*p*	BSAO	1998VAN/VAN

Correlated heat capacities (45.182.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936KIN/GAR	312.1	1	3.00	#	0.234	5.64−1	0.70	5.64−1	1
2004VAN/OON	330.0–350.0	3	0.20		0.247	4.07−2	0.05	−7.78−4	1

Parameters of regression polynomial (45.182.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	5	4	0.345	4.02−1	0.50	1.40−1	2		
T/K		A_1		A_2		A_3		A_4	Uncert.
312.1–350.0		4.860 26+1		9.945 02					III

Deviation plot for Methyl nonadecanoate (45–182) is given in Fig. 133.

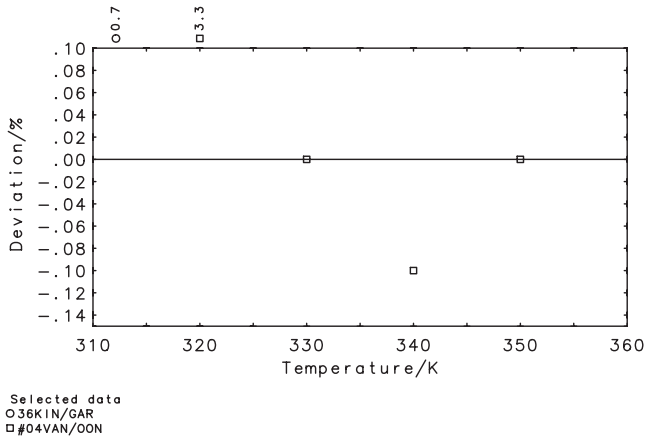

FIG. 133. Deviation plot for methyl nonadecanoate (45-182).

6.5.5.46. Ethyl nonadecanoate (45-183)

Name:	Ethyl nonadecanoate
Formula:	$C_{21}H_{42}O_2$
CAS-RN:	18281-04-4
Group No:	45-183

Experimental heat capacities (45.183.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		301.15	2.09	n/a	n/a	n/a	*p*	DSIO	1924GAR/RAN

6.5.5.47. Methyl eicosanoate (45-184)

Name:	Methyl eicosanoate
Formula:	$C_{21}H_{42}O_2$
CAS-RN:	1120-28-1
Group No:	45-184

Experimental heat capacities (45.184.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		319.1	1		n/a	n/a	n/a	*p*	DSIO	1924GAR/RAN
2004VAN/OON		330.0–350.0	3	S	0.20	99.1	chrom	*p*	BSAO	1998VAN/VAN

Correlated heat capacities (45.184.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1936KIN/GAR	319.1	1	3.00	#	0.090	2.30−1	0.27	2.30−1	1
2004VAN/OON	330.0–350.0	3	0.20		0.017	2.89−3	0.00	−3.31−4	0

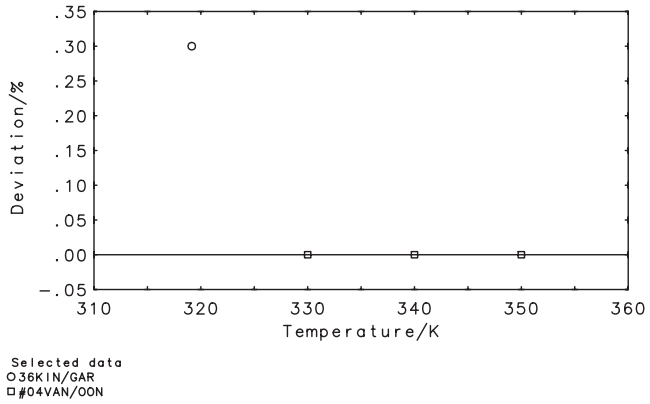

FIG. 134. Deviation plot for methyl eicosanoate (45-184).

Parameters of regression polynomial (45.184.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.094	2.30−1	0.27	5.73−2	1

T/K	A_1	A_2	A_3	A_4	Uncert.
319.1–350.0	2.040 52+2	−7.958 43+1	1.327 00+1		II

Deviation plot for Methyl eicosanoate (45–184) is given in Fig. 134.

6.5.5.48. Methyl docosanoate (45-185)

Name:	Methyl docosanoate
Formula:	$C_{23}H_{46}O_2$
CAS-RN:	929-77-1
Group No:	45-185

Experimental heat capacities (45.185.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1936KIN/GAR		325.15	2.25	n/a	n/a	n/a	*p*	DSIO	1924GAR/RAN

6.5.5.49. 1,2,3,4,5,6-Benzenehexayl ester pentanoic acid (45-186)

Name:	1,2,3,4,5,6-Benzenehexayl ester pentanoic acid
Formula:	$C_{36}H_{54}O_{12}$
CAS-RN:	65201-68-5
Group No:	45-186

Experimental heat capacities (45.186.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001ASA/SOR		381.3–389.1	5	n/a	99.94	melpt	*p*	BSAO	1992SOR/KAJ

Parameters of regression polynomial (45.186.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.017	2.87−2	0.02	6.10−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
381.3–389.1	8.610 74+1	2.06704+1			II

6.5.5.50. 2-[(1-Oxohexadecyl)oxy]-1-[[(1-oxohexadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid (45-187)

Name: 2-[(1-Oxohexadecyl)oxy]-1-[[(1-oxohexadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid

Formula: $C_{53}H_{100}O_6$
CAS-RN: 2190-25-2
Group No: 45-187

Experimental heat capacities (45.187.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000MOR/KAM		333.1–453.1	7	1.00	n/a	n/a	p	BDHT	1995MOR/IDR1

Parameters of regression polynomial (45.187.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.000	1.37−5	0.00	−4.36−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
333.1–453.1	1.326 19+2	2.505 79+1			IV

6.5.5.51. 1-[[(1-Oxohexadecyl)oxy]methyl]-2-[(1-oxooctadecyl)oxy]ethyl ester (9*Z*)-9-octadecenoic acid (45-188)

Name: 1-[[(1-Oxohexadecyl)oxy]methyl]-2-[(1-oxooctadecyl)oxy]ethyl ester (9*Z*)-9-octadecenoic acid

Formula: $C_{55}H_{104}O_6$
CAS-RN: 2190-27-4
Group No: 45-188

Experimental heat capacities (45.188.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000MOR/KAM		333.1–453.1	7	1.00	n/a	n/a	p	BDHT	1995MOR/IDR1

Parameters of regression polynomial (45.188.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.001	3.50−3	0.00	−1.09−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
333.1–453.1	1.399 33+2	2.484 33+1			IV

6.5.5.52. 1,2,3-Propanetriyl ester (9*E*,9′*E*,9″*E*)-9-octadecenoic acid (45-189)

Name: 1,2,3-Propanetriyl ester (9*E*,9′*E*,9″*E*)-9-octadecenoic acid

Formula: $C_{57}H_{104}O_6$
CAS-RN: 537-39-3
Group No: 45-189

Experimental heat capacities (45.189.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003VAN/VAN2		319.0–339.2	11	0.50	96.66	melpt	p	BSAO	2002VAN/VAN1

Parameters of regression polynomial (45.189.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	11	11	0.158	1.81−1	0.08	2.30−4	0

T/K	A_1	A_2	A_3	A_4	Uncert.
319.0–339.2	1.447 21+2	2.585 60+1	II		

6.5.5.53. 1,2,3-Propanetriyl ester (9*Z*)-9-octadecenoic acid (45-190)

Name: 1,2,3-Propanetriyl ester (9*Z*)-9-octadecenoic acid

Formula: $C_{57}H_{104}O_6$
CAS-RN: 122-32-7
Group No: 45-190

Experimental heat capacities (45.190.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000MOR/KAM		333.1–453.1	7	1.00	n/a	n/a	p	BDHT	1995MOR/IDR1

Parameters of regression polynomial (45.190.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.000	1.37−5	0.00	−4.36−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
333.1–453.1	1.508 39+2	2.129 90+1	IV		

6.5.5.54. 2-[(1-Oxooctadecyl)oxy]-1-[[(1-oxooctadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid (45-191)

Name: 2-[(1-Oxooctadecyl)oxy]-1-[[(1-oxooctadecyl)oxy]methyl]ethyl ester (9*Z*)-9-octadecenoic acid

Formula: $C_{57}H_{108}O_6$
CAS-RN: 2846-04-0
Group No: 45-191

Experimental heat capacities (45.191.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000MOR/KAM		333.1–453.1	7	1.00	n/a	n/a	p	BDHT	1995MOR/IDR1

Parameters of regression polynomial (45.191.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	7	7	0.000	1.37−5	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
333.1–453.1		1.477 49+2		2.481 93+1				IV

6.5.5.55. 1,2,3,4,5,6-Benzenehexayl ester nonanoic acid (45-192)

Name: 1,2,3,4,5,6-Benzenehexayl ester nonanoic acid

Formula: $C_{60}H_{102}O_{12}$
CAS-RN: 65201-72-1
Group No: 45-192

Experimental heat capacities (45.192.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003ASA/SOR		355.2–389.0	16	n/a	99.41	melpt	p	BSAO	1983YOS/SOR1

Parameters of regression polynomial (45.192.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	16	16	0.027	7.52−2	0.03	−6.01−4	−1		
T/K		A_1		A_2		A_3		A_4	Uncert.
355.2–389.0		−8.668 21+3		7.510 50+3		−2.089 12+3		1.927 13+2	II

6.5.5.56. 1,2,3,4,5,6-Benzenehexayl ester decanoic acid (45-193)

Name: 1,2,3,4,5,6-Benzenehexayl ester decanoic acid

Formula: $C_{66}H_{114}O_{12}$
CAS-RN: 65201-73-2
Group No: 45-193

Experimental heat capacities (45.193.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003ASA/SOR		364.1–388.8	10	n/a	99.73	melpt	*p*	BSAO	1983YOS/SOR1

Parameters of regression polynomial (45.193.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.104	3.26−1	0.10	2.37−3	0

T/K	A_1	A_2	A_3	A_4	Uncert.
364.1–388.8	2.223 69+4	−1.696 68+4	4.379 69+3	−3.771 66+2	II

6.5.6. Sub group 46: heterocyclic oxygen compounds

6.5.6.1. 1,3-Dioxolane (46-004)

Name: 1,3-Dioxolane

Formula: $C_3H_6O_2$
CAS-RN: 646-06-0
Group No: 46-004

Experimental heat capacities (46.4.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1969CLE/MEL4		175.9–300.0	16	S	n/a	99.93	melpt	sat	BSAO	1968CLE/MEL
1976CON/GIA		298.1	1		n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1988ING		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1999BRO/CAL1		298.1	1		n/a	99.8	anal	*p*	FSIT	1971PIC/LED
1999BRO/CAL2		298.1	1		n/a	99.8	chrom	*p*	FSIT	1971PIC/LED
2004BRO/PIN		298.1	1		−1.0	99.0	anal	*p*	FSIT	1971PIC/LED

6.5.6.2. 2,3-Dihydrofuran (46-007)

Name: 2,3-Dihydrofuran

Formula: C_4H_6O
CAS-RN: 1191-99-7
Group No: 46-007

Experimental heat capacities (46.7.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1989STE/CHI3		298.1	1		1.00	99.95	chrom	*p*	BDHT	1989KNI/ARC
2002STE/CHI6		300.0–520.0	12	S	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

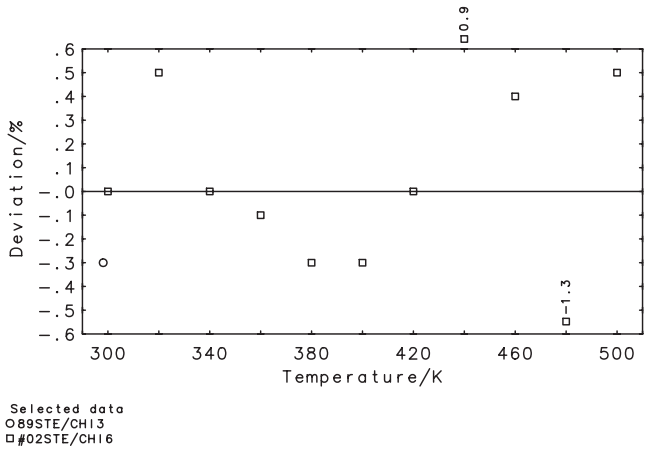

FIG. 135. Deviation plot for 2,3-dihydrofuran (46-007).

Correlated heat capacities (46.7.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1989STE/CHI3	298.1	1	1.00	0.299	4.39−2	0.30	−4.39−2	−1
2002STE/CHI6	300.0–500.0	11	1.00	0.544	1.18−1	0.54	5.61−3	−1

Parameters of cubic spline polynomials (46.7.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	13	12	0.691	1.49−1	0.69	1.48−3	−2
sat	13	12	0.483	9.74−2	0.48	6.27−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–420.0	2.798 42+1	−1.583 62+1	5.176 35	−4.542 56−1	III
420.0–500.0	−6.815 01+2	4.909 39+2	−1.154 84+2	9.121 99	III
298.1–420.0	2.243 19+1	−1.150 55+1	4.102 21	−3.720 59−1	II
420.0–500.0	−3.919 40+2	2.844 74+2	−6.636 91+1	5.220 91	III

Parameters of quasipolynomial equation (46.7.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	13	13	0.271	5.55−2	0.27	9.43−5	1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
298.1–520.0	525.00	−1.241 01	2.715 13−1	−1.023 19	3.717 33+1	−2.568 92+1	6.773 68	II

Deviation plot for 2,3–Dihydrofuran (46–007) is given in Fig. 135.

6.5.6.3. Tetrahydrofuran (46-009)

Name:	Tetrahydrofuran
Formula:	C_4H_8O
CAS-RN:	109-99-9
Group No:	46-009

Experimental heat capacities (46.9.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1976BON/CER		298.1	1	n/a	n/a	n/a	*p*	BSIO	1976BON/CER
1976CON/GIA		298.1	1	n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1978LEB/RAB2	N	161.6–322.6	50	0.20	99.8	melpt	*p*	BSAO	1976LEB/LIT
1979KIY/DAR		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1985COS/PAT9		283.1–313.1	3	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1988ING		298.1	1	n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994CON/GIA1		298.1	1	n/a	n/a	n/a	*p*	FSIT	1988CON/GIA
1994CON/GIA2		298.1	1	n/a	99.5	anal	*p*	FSIT	1988CON/GIA
1997CON/GIA		298.1	1	n/a	n/a	n/a	*p*	FSIT	1988CON/GIA
1998CON/GIA		298.1	1	0.50	99.5	chrom	*p*	FSIT	1988CON/GIA
1999BRO/CAL1		298.1	1	n/a	99.9	anal	*p*	FSIT	1971PIC/LED
2002BRO/PIN		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
2006DIE/GME		180.1–325.1	30	3.00	99.9	chrom	*p*	BDHT	2004KIM/SHI

Reference	Notes
1978LEB/RAB2	same data in 1979LEB/LIT and smoothed data in 1977LEB/LIT1

6.5.6.4. 1,3-Dioxane (46-010)

Name:	1,3-Dioxane
Formula:	$C_4H_8O_2$
CAS-RN:	505-22-6
Group No:	46-010

Experimental heat capacities (46.10.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1976CON/GIA		298.1	1	n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1988ING		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1995TAK/OGA		298.1	1	1.00	99.96	chrom	*p*	FSIO	1985OGA
2000TAK/TAM		298.1	1	n/a	99.99	chrom	*p*	FSIO	1985OGA

6.5.6.5. 1,4-Dioxane (46-011)

Name:	1,4-Dioxane
Formula:	$C_4H_8O_2$
CAS-RN:	123-91-1
Group No:	46-011

Experimental heat capacities (46.11.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1929HER/LOR		296.1	1		n/a	n/a	n/a	*p*	DSIO	1922HER/SCH
1933ROT/MEY1		291.1	1		n/a	n/a	n/a	*p*	DSIO	1933ROT/MEY2
1934JAC/PAR		288.7–298.2	3		n/a	n/a	n/a	*p*	BSIO	1925PAR
1952STA/AMI		313.1	1		n/a	n/a	n/a	*p*	BSIO	1952STA/AMI
1961ROU		296.9–313.7	14		n/a	n/a	n/a	*p*	BSAO	1961ROU
1971DES/BHA		298.1–318.1	3	S	n/a	n/a	n/a	*p*	BSIO	1958MUR/VAN
1971KHA/SUB		298.1–313.1	2		n/a	n/a	n/a	*p*	BSIO	1964MOE/THO
1976BON/CER		298.1	1		n/a	n/a	n/a	*p*	BSIO	1976BON/CER
1976CON/GIA		298.1	1		n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1979MUR/SUB		298.1	1		n/a	n/a	n/a	*p*	BSIO	1964MOE/THO
1984GRO/ING		298.1	1		0.30	99.5	melpt	*p*	FSIT	1971PIC/LED
1984ING/GRO		298.1	1		0.30	99.5	chrom	*p*	FSIT	1971PIC/LED
1988ING		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1989BAR/KOO2		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1991GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1991TRE/COS		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1993GRO/ROU		298.1	1		n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1994GRO/ROU		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED
1995TAK/OGA		298.1	1		1.00	99.97	chrom	*p*	FSIO	1985OGA
1999BRO/CAL1		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
2000TAK/TAM		298.1	1		n/a	99.99	chrom	*p*	FSIO	1985OGA
2003BRO/PIN2		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED

6.5.6.6. Tetrahydropyran (46-014)

Name:	Tetrahydropyran
Formula:	$C_5H_{10}O$
CAS-RN:	142-68-7
Group No:	46-014

Experimental heat capacities (46.14.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1964MOE/THO		297.6–327.5	4	S	0.50	n/a	n/a	*p*	BSIO	1964MOE/THO
1976CON/GIA		298.1	1		n/a	n/a	n/a	*p*	BDCT	1976CON/GIA
1984ING/GRO		298.1	1		0.30	99.	chrom	*p*	FSIT	1971PIC/LED
1988ING		298.1	1		n/a	99.	anal	*p*	FSIT	1971PIC/LED
1999BRO/CAL1		298.1	1		n/a	99.	chrom	*p*	FSIT	1971PIC/LED
2003BRO/PIN1		298.1	1		n/a	99.0	anal	*p*	FSIT	1971PIC/LED

Correlated heat capacities (46.14.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1964MOE/THO	297.6–327.5	4	0.50		1.263	1.16−1	0.63	6.92−2	2
1984ING/GRO	298.1	1	0.30		0.451	2.44−2	0.14	−2.44−2	−1
1988ING	298.1	1	0.50	#	0.794	7.12−2	0.40	−7.12−2	−1
1999BRO/CAL1	298.1	1	0.50	#	0.808	7.25−2	0.40	−7.25−2	−1
2003BRO/PIN1	298.1	1	0.50	#	0.646	5.80−2	0.32	−5.80−2	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1976CON/GIA	(1.11, 6.56, −1.11, −1)

Parameters of regression polynomial (46.14.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	9	8	1.175	1.07−1	0.58	6.33−3	−2
T/K		A_1		A_2	A_3	A_4	Uncert.
297.6–327.5		2.970 67		5.046 59			IV

Deviation plot for Tetrahydropyran (46–014) is given in Fig. 136.

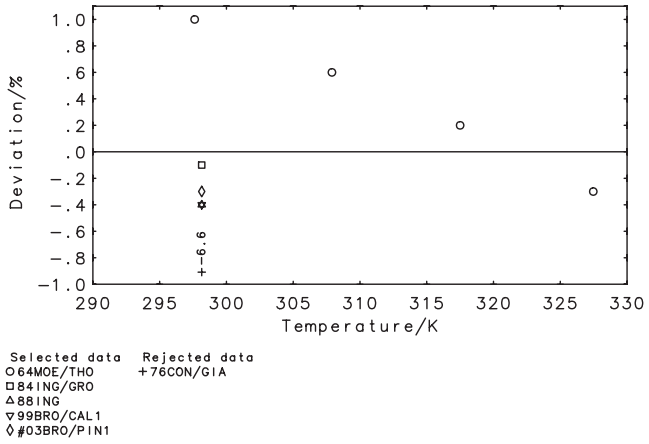

FIG. 136. Deviation plot for tetrahydropyran (46-014).

6.5.6.7. Dibenzo[*b*,*e*][1,4]dioxin (46-032)

Name:	Dibenzo[*b*,*e*][1,4]dioxin
Formula:	$C_{12}H_8O_2$
CAS-RN:	262-12-4
Group No:	46-032

Experimental heat capacities (46.32.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001LEB/SMI		390.6–415.0	4	S	1.50	n/a	n/a	*p*	BDHT	1985GUS/DAV

Parameters of regression polynomial (46.32.3)

Type	nTot	nPts	s_w	*s*/R	s_r/%	s_b/R	+/−
p	4	4	0.038	2.04−2	0.06	9.54−6	0
T/K		A_1		A_2	A_3	A_4	Uncert.
390.6–415.0		−1.481 84+1		1.247 96+1			IV

6.5.6.8. 6,7,9,10,12,13,20,21,23,24,26,27-Dodecahydrodibenz[*b*,*n*][1,4,7,10,13,16,19,22]octaoxacyclotetracosin (46-033)

Name:	6,7,9,10,12,13,20,21,23,24,26,27-Dodecahydrodibenz[*b*,*n*][1,4,7,10,13,16,19,22]octaoxacyclotetracosin
Formula:	$C_{24}H_{32}O_8$
CAS–RN:	14174-09-5
Group No:	46-033

Experimental heat capacities (46.33.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004BYK/LEB	N	375.5–480.0	12 S	0.50	98.0	anal	*p*	BDHT	1985GUS/DAV

Reference	Notes
2004BYK/LEB	only figure in 2002LEB/BYK; data from authors

Parameters of regression polynomial (46.33.3)

Type	nTot	nPts	s_w	*s*/R	s_r/%	s_b/R	+/−
p	12	12	0.067	3.81−2	0.03	2.16−5	0
T/K		A_1		A_2	A_3	A_4	Uncert.
375.5–480.0		9.607 30+1		4.319 11			II

6.5.7. Sub group 47: miscellaneous oxygen compounds

6.5.7.1. 1,3-Dioxolan-2-one (47-002)

Name:	1,3-Dioxolan-2-one
Formula:	$C_3H_4O_3$
CAS-RN:	96-49-1
Group No:	47-002

Experimental heat capacities (47.2.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1958PEP		323.1	1	n/a	n/a	n/a	*p*	n/a	n/a
1973VAS/KOR	N	309.5–350.0	5 S	n/a	99.83	melpt	*p*	BSAO	1977KU/COM
2004CHE/CLE		383.1–398.1	4	2.50	99.9	chrom	*p*	BDHT	2004CHE/CLE
2004DIN		311.0–323.0	eqn	n/a	n/a	n/a	*p*	BDHT	1998SAL/FER

Reference	Notes
1973VAS/KOR	selected data in 1974VAS/KOR and 1975VAS/VAS

Correlated heat capacities (47.2.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1973VAS/KOR	309.5–350.0	5	1.00	#	0.202	3.47−2	0.20	−4.33−3	1
2004CHE/CLE	383.1–398.1	4	2.50		0.266	1.25−1	0.66	3.66−2	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1958PEP	(7.48−1, 4.65, −7.48−1, −1)	2004DIN	(1.65+1, >100, −1.65+1, −10)

Parameters of regression polynomial (47.2.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	20	9	0.285	1.07−1	0.57	1.38−2	1

T/K	A_1	A_2	A_3	A_4	Uncert.
309.5–398.1	3.055 22+1	−1.024 26+1	1.856 01		V

Deviation plot for 1,3–Dioxolan—2–one (47–002) is given in Fig. 137.

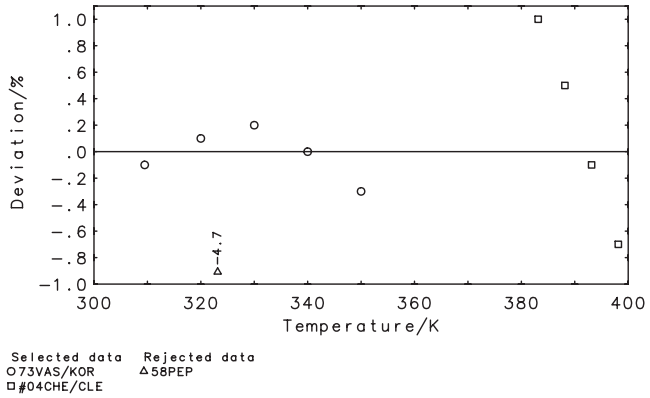

FIG. 137. Deviation plot for 1,3-dioxolan-2-one (47-002).

6.5.7.2. 2-Methoxyethanol (47-004)

Name:	2-Methoxyethanol
Formula:	$C_3H_8O_2$
CAS-RN:	109-86-4
Group No:	47-004

Experimental heat capacities (47.4.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1952CUR/JOH	N	293.1	1	n/a	n/a	n/a	p	n/a	n/a
1973KUS/SUU		298.1	1	n/a	n/a	n/a	p	DDCT	1971KON/SUU
1978ROU/PER2		298.1	1	n/a	99.	chrom	p	FSIT	1971PIC/LED
1989COB/GAR		298.1	1	n/a	99.5	anal	p	FSIT	1971PIC/LED
1991SVO/ZAB2		300.6–328.3	7	0.50	99.95	chrom	p	BSAO	1991SVO/ZAB1
1993PAG/HUO1		298.1–313.1	2	n/a	99.7	anal	p	FSIT	1971PIC/LED
1997NIS/TAB		293.1–303.1	3	n/a	99.97	chrom	p	FSIO	1985OGA
1998CON/GIA		298.1	1	0.50	99.5	chrom	p	FSIT	1988CON/GIA

Reference	Notes
1952CUR/JOH	technical product, purity in question

Correlated heat capacities (47.4.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1973KUS/SUU	298.1	1	0.30	#	0.714	4.51−2	0.21	−4.51−2	−1
1978ROU/PER2	298.1	1	0.50	#	1.276	1.35−1	0.64	1.35−1	1
1991SVO/ZAB2	300.6–328.3	7	0.50		0.432	4.62−2	0.22	9.67−3	−1
1997NIS/TAB	293.1–303.1	3	1.50	#	0.270	8.47−2	0.40	−6.39−2	−1
1998CON/GIA	298.1	1	0.50		0.497	5.23−2	0.25	−5.23−2	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1952CUR/JOH	(4.70−1, 2.30, −4.70−1, −1)	1989COB/GAR	(3.42−1, 1.65, −3.42−1, −1)
1993PAG/HUO1	(1.50, 6.37, 1.28, 2)		

Parameters of regression polynomial (47.4.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	17	13	0.625	7.72−2	0.37	−6.62−3	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
293.1–328.3	2.592 50+1	−6.577 50	1.661 15		III

Deviation plot for Methoxyethanol (47–004) is given in Fig. 138.

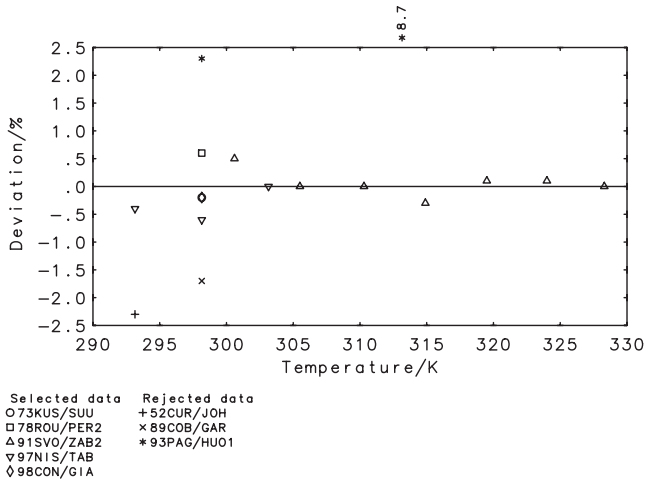

FIG. 138. Deviation plot for 2-methoxyethanol (47-004).

6.5.7.3. 4-Methyl-1,3-dioxolan-2-one (47-007)

Name:	4-Methyl-1,3-dioxolan-2-one
Formula:	$C_4H_6O_3$
CAS-RN:	108-32-7
Group No:	47-007

Experimental heat capacities (47.7.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1958PEP		323.1	1	n/a	n/a	n/a	*p*	n/a	n/a
1976MAS/PET	N	235.5–325.8	13	5.00	n/a	n/a	*p*	BDHT	1966PER/COM
1976VAS/KOR	N	226.7–416.3	93	n/a	99.32	melpt	*p*	BSAO	1977KU/COM
1991WIL/JIM		298.1	1	n/a	99.	anal	*p*	FSIT	1971PIC/LED
1993ANG/BOE	N	229.0	1	n/a	99.	anal	*p*	BDHT	1969PER/COM
1994FUJ/OGU		222.1–300.9	37	0.30	99.974	melpt	sat	BSAO	1993FUJ/OGU1
1997COM/RIG		288.1–313.1	3	n/a	n/a	n/a	*p*	BDHT	1995DIO/MAN
1997RIG/COM		288.1–313.1	3	1.00	99.7	chrom	*p*	BDHT	1995DIO/MAN
2004CHE/CLE		303.1–393.1	10	2.50	99.9	chrom	*p*	BDHT	2004CHE/CLE
2004DIN		220.0–323.0	eqn	n/a	n/a	n/a	*p*	BDHT	1998SAL/FER

Reference	Notes
1976MAS/PET	data from a graph only
1976VAS/KOR	smoothed data in 1974VAS/KOR
1993ANG/BOE	data from a graph only

6.5.7.4. 2,2′-Oxybis(ethanol) (47-009)

Name:	2,2′-Oxybis(ethanol)
Formula:	$C_4H_{10}O_3$
CAS-RN:	111-46-6
Group No:	47-009

Experimental heat capacities (47.9.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1952CUR/JOH	N	293.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1959DEA/EVA	N	303.1–473.1	3	S	n/a	n/a	n/a	*p*	n/a	n/a
1979STE/TAM		273.1–513.2	14	S	n/a	99.9	chrom	sat	BDHT	1969PER/COM
1982ZAR		298.0–363.0	3		0.60	99.5	chrom	*p*	BDCT	1982ZAR
1988MUK/ZAR		300.5–422.3	6		n/a	n/a	n/a	*p*	BDCT	1982ZAR

Reference	Notes
1952CUR/JOH	technical product, purity in question
1959DEA/EVA	data of Shell Development Company Emeryville, California

6.5.7.5. 2-Butoxyethanol (47-023)

Name:	2-Butoxyethanol
Formula:	$C_6H_{14}O_2$
CAS-RN:	111-76-2
Group No:	47-023

Experimental heat capacities (47.23.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1952CUR/JOH	N	293.1	1		n/a	n/a	n/a	*p*	n/a	n/a
1959ONK		298.1–373.1	16	S	n/a	n/a	n/a	*p*	BSAO	1959ONK
1973KUS/SUU		298.1	1		0.10	n/a	n/a	*p*	DDCT	1971KON/SUU
1978ROU/PER2		277.1–328.1	5		n/a	99.	chrom	*p*	FSIT	1971PIC/LED
1989COB/GAR		298.1	1		n/a	98.	anal	*p*	FSIT	1971PIC/LED
1999TAM/OSA		298.1	1		n/a	99.88	chrom	*p*	FSIO	1985OGA
2000ATA/KAW		210.0–300.0	11	S	n/a	99.86	melpt	*p*	BSAO	1974ATA/CHI

Reference	Notes
1952CUR/JOH	technical product, purity in question

Correlated heat capacities (47.23.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1959ONK	298.1–373.1	16	0.50	#	0.486	8.58−2	0.24	−2.06−2	−3
1973KUS/SUU	298.1	1	0.10		0.823	2.70−2	0.08	2.70−2	1
1978ROU/PER2	277.1–328.1	5	0.50	#	1.443	2.38−1	0.72	−5.67−2	−1
1999TAM/OSA	298.1	1	2.00	#	0.975	6.52−1	1.95	6.52−1	1
2000ATA/KAW	210.0–300.0	11	1.00	#	0.268	8.57−2	0.27	−2.77−2	−1

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1952CUR/JOH	(2.15, 6.20, 2.15, 1)	1989COB/GAR	(4.73−1, 1.46, −4.73−1, −1)

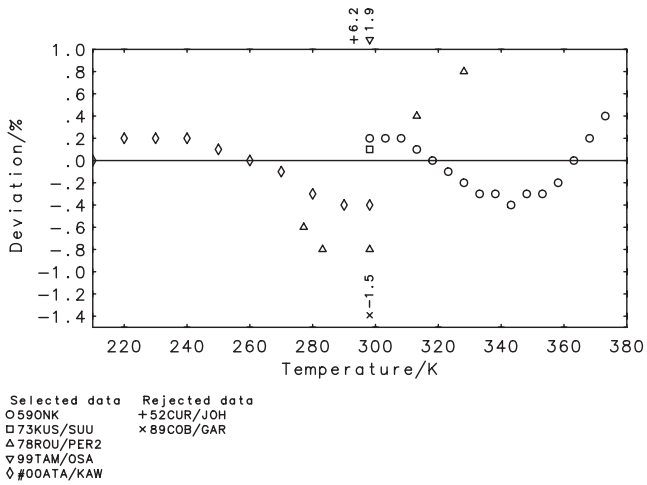

FIG. 139. Deviation plot for 2-butoxyethanol (47-023).

Parameters of regression polynomial (47.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	36	34	0.744	1.74−1	0.52	−7.01−3	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
210.0–373.1	6.051 39+1	−3.894 16+1	1.476 91+1	−1.617 81	IV

Deviation plot for 2–Butoxyethanol (47–023) is given in Fig. 139.

6.5.7.6. 2,2′-[1,2-Ethanediylbis(oxy)]bis(ethanol) (47-025)

Name:	2,2′-[1,2-Ethanediylbis(oxy)]bis(ethanol)
Formula:	$C_6H_{14}O_4$
CAS-RN:	112-27-6
Group No:	47-025

Experimental heat capacities (47.25.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1952CUR/JOH	N	293.1	1		n/a	n/a	n/a	p	n/a	n/a
1979STE/TAM		273.1–533.2	15	S	n/a	99.9	chrom	sat	BDHT	1969PER/COM
1982ZAR		298.0–363.0	3		0.60	98.5	chrom	p	BDCT	1982ZAR
2002STE/CHI3		303.0–553.0	eqn		1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1952CUR/JOH	technical product, purity in question

Correlated heat capacities (47.25.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1979STE/TAM	273.1–533.2	15	2.00	#	1.353	1.30	2.70	7.30−1	7
1982ZAR	298.0–363.0	3	0.60		0.886	2.23−1	0.53	8.13−2	1
2002STE/CHI3	303.0–552.6	25	1.00		0.374	1.73−1	0.37	−1.24−1	−15

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1952CUR/JOH	(1.25−1, 0.32, −1.25−1, −1)

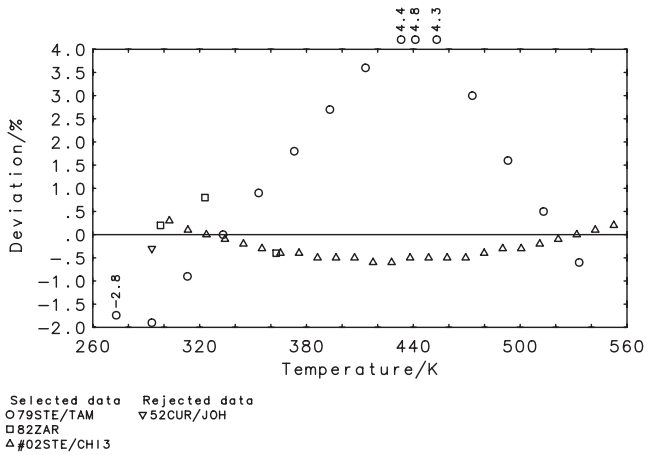

FIG. 140. Deviation plot for 2,2′-[1,2-Ethanediylbis(oxy)]bis(ethanol) (47-025).

Parameters of regression polynomial (47.25.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	44	43	0.912	8.08−1	1.69	1.88−1	−7
sat	44	43	0.912	8.08−1	1.69	1.88−1	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
273.1–552.6	2.189 77+1	6.783 96	−2.309 78−1		IV
273.1–552.6	2.189 32+1	6.786 48	−2.313 22−1		IV

Parameters of quasi-polynomial equation (47.25.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	44	43	1.192	7.23−1	1.51	2.37−2	−5

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
273.1–552.6	770.00	2.311 16+1	1.710 70	1.474 97+1	8.878 08+1	−6.483 88	1.547 38−1	IV

Deviation plot for 2,2′-[1,2-Ethanediylbis(oxy)]bis(ethanol) (47-025) is given in Fig. 140.

6.5.7.7. Phenyl ester 2-hydroxybenzoic acid (47-041)

Name:	Phenyl ester 2-hydroxybenzoic acid
Formula:	$C_{13}H_{10}O_3$
CAS-RN:	118-55-8
Group No:	47-041

Experimental heat capacities (47.41.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1913CAM	N	317.3	1	n/a	n/a	n/a	p	BSIO	1913CAM
2002HAN/HIK		318.0–353.7	13	0.20	99.95	melpt	p	BSAO	1993FUJ/OGU1

Reference	Notes
1913CAM	Err/% of 0.5% (information in 1929WAS)

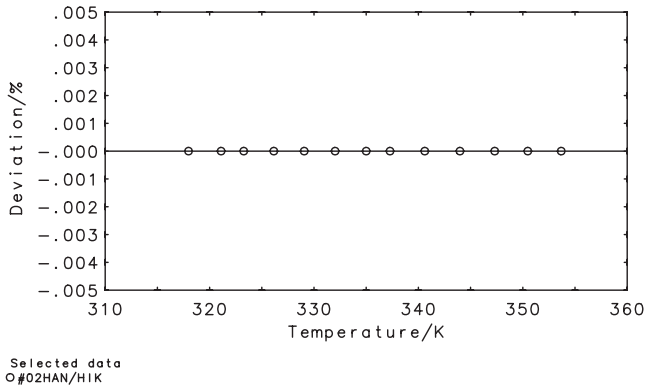

FIG. 141. Deviation plot for phenyl ester 2-hydroxybenzoic acid (47-041).

Correlated heat capacities (47.41.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002HAN/HIK	318.0–353.7	13	0.20	0.053	4.42−3	0.01	2.05−6	1

Parameters of regression polynomial (47.41.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	14	13	0.058	4.81−3	0.01	2.05−6	1

T/K	A_1	A_2	A_3	A_4	Uncert.
318.0–353.7	2.039 24+1	6.297 25			II

Deviation plot for Phenyl ester 2-hydroxybenzoic acid (47-041) is given in Fig. 141.

6.5.7.8. 1,4-Dioxan-2-one (47-076)

Name:	1,4-Dioxan-2-one
Formula:	$C_4H_6O_3$
CAS-RN:	3041-16-5
Group No:	47-076

Experimental heat capacities (47.76.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference	
1995LEB/BYK1	N	301.7–450.0	16	S	n/a	99.47	melpt	p	BDHT	1985GUS/DAV

Reference	Notes
1995LEB/BYK1	graph only in the article; smoothed data by authors

Parameters of regression polynomial (47.76.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	16	16	0.457	4.99−2	0.23	1.66−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
301.7–450.0	7.996 00+1	−5.112 51+1	1.392 75+1	−1.170 05	II

6.5.7.9. 4-Hydroxymethyl-1,3-dioxolan-2-one (47-077)

Name:	4-Hydroxymethyl-1,3-dioxolan-2-one
Formula:	$C_4H_6O_4$
CAS-RN:	931-40-8
Group No:	47-077

Experimental heat capacities (47.77.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004CHE/CLE		283.1–373.1	10	2.50	98.9	chrom	p	BDHT	2004CHE/CLE

Parameters of regression polynomial (47.77.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.126	8.33−2	0.32	4.43−4	2
T/K		A_1		A_2	A_3	A_4	Uncert.
283.1–373.1		1.970 26+1		2.015 80			IV

6.5.7.10. 4-Ethyl-1,3-dioxolan-2-one (47-078)

Name:	4-Ethyl-1,3-dioxolan-2-one
Formula:	$C_5H_8O_3$
CAS-RN:	4437-85-8
Group No:	47-078

Experimental heat capacities (47.78.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004CHE/CLE		283.1–373.1	10	2.50	99.7	chrom	p	BDHT	2004CHE/CLE

Parameters of regression polynomial (47.78.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.063	3.84−2	0.16	9.82−5	0
T/K		A_1		A_2	A_3	A_4	Uncert.
283.1–373.1		1.465 03+1		3.004 49			IV

6.5.7.11. 2-(1,1-Dimethylethoxy)ethanol (47-079)

Name:	2-(1,1-Dimethylethoxy)ethanol
Formula:	$C_6H_{14}O_2$
CAS-RN:	7580-85-0
Group No:	47-079

Experimental heat capacities (47.79.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000ATA/KAW		230.0–300.0	9	S	n/a	99.63	melpt	p	BSAO	1974ATA/CHI

Parameters of regression polynomial (47.79.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	9	9	0.178	5.36−2	0.18	2.60−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
230.0–300.0	1.220 81+1	6.916 93			III

6.5.7.12. 4,5,6,7-Tetrahydro-1,3-isobenzofurandione (47-080)

Name: 4,5,6,7-Tetrahydro-1,3-isobenzofurandione

Formula: $C_8H_8O_3$
CAS-RN: 2426-02-0
Group No: 47-080

Experimental heat capacities (47.80.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004LV/TAN		346.5–360.3	8	0.30	99.28	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (47.80.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	8	8	0.121	1.22−2	0.04	9.54−7	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
346.5–360.3	1.298 07+2	−6.284 61+1	1.008 07+1		II

6.5.7.13. 3*a*,4,7,7*a*-Tetrahydro-5-methyl-1,3-isobenzofurandione (47-081)

Name: 3*a*,4,7,7*a* -Tetrahydro-5-methyl-1,3-isobenzofurandione

Formula: $C_9H_{10}O_3$
CAS-RN: 3425-89-6
Group No: 47-081

Experimental heat capacities (47.81.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005LV/TAN		339.3–360.1	12	0.30	99.4	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (47.81.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.229	2.63−2	0.07	−1.65−3	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
339.3–360.1	1.458 80+4	−1.233 04+4	3.478 15+3	−3.265 61+2	II

6.5.7.14. 2-[2-(Hexyloxy)ethoxy]ethanol (47-082)

Name:	2-[2-(Hexyloxy)ethoxy]ethanol
Formula:	$C_{10}H_{22}O_3$
CAS-RN:	112-59-4
Group No:	47-082

Experimental heat capacities (47.82.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005PIE/TKA2		275.1–328.1	7	1.50	98.0	anal	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (47.82.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.037	2.81−2	0.06	3.11−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
275.1–328.1	3.171 99+1	6.446 68			IV

6.5.7.15. 1′-Hydroxy[1,1′-bicyclohexyl]-2-one (47-083)

Name:	1′-Hydroxy[1,1′-bicyclohexyl]-2-one
Formula:	$C_{12}H_{20}O_2$
CAS-RN:	28746-99-8
Group No:	47-083

Experimental heat capacities (47.83.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006SHE/KAB	N	306.8–370.0	8	S	2.00	99.82	melpt	p	BDHT	1992KAB/KOZ
2006SHE/KAB		308.3–311.7	3		0.40	99.82	melpt	sat	BDHT	1993DIK/KAB

Reference	Notes
2006SHE/KAB	same data in 2004BLO/KAB

Correlated heat capacities (47.83.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2006SHE/KAB	306.8–370.0	8	2.00	0.017	1.55−2	0.03	−1.17−3	0
2006SHE/KAB	308.3–311.7	3	0.40	0.225	3.80−2	0.09	1.91−4	1

Parameters of regression polynomial (47.83.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	11	11	0.139	2.80−2	0.07	−7.99−4	1	

T/K	A_1	A_2	A_3	A_4	Uncert.
306.8–370.0	7.443 32+1	−2.895 53+1	5.999 64		II

Deviation plot for 1′-Hydroxy[1,1′-bicyclohexyl]-2-one (47-083) is given in Fig. 142.

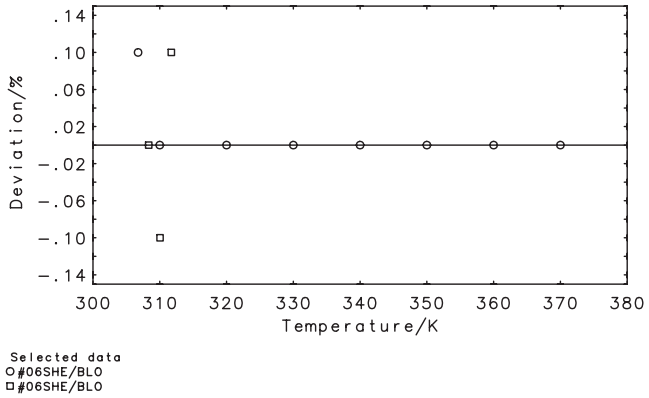

FIG. 142. Deviation plot for 1′-hydroxy[1,1′-bicyclohexyl]-2-one (47-083).

6.5.7.16. 3,6,9,12-Tetraoxadecan-1-ol (47-084)

Name:	3,6,9,12-Tetraoxadecan-1-ol
Formula:	$C_{14}H_{30}O_5$
CAS-RN:	39619-69-7
Group No:	47-084

Experimental heat capacities (47.84.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006PIE/TKA		280.0–333.0	7	0.15	99.0	anal	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (47.84.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	7	7	0.805	8.74−2	0.12	1.95−4	0		
T/K		A_1		A_2		A_3		A_4	Uncert.
280.0–333.0		9.252 85+2		−8.504 81+2		2.802 37+2		−3.050 61+1	IV

6.5.7.17. 3,6,9,12,15-Pentaoxaheneicosan-1-ol (47-085)

Name:	3,6,9,12,15-Pentaoxaheneicosan-1-ol
Formula:	$C_{16}H_{34}O_6$
CAS-RN:	86674-95-5
Group No:	47-085

Experimental heat capacities (47.85.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005PIE/TKA1		283.0–338.0	7	0.15	99.0	anal	p	BDCT	2000ERN/CHO

Parameters of regression polynomial (47.85.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	7	7	0.255	3.26−2	0.04	1.42−5	−1	
T/K		A_1		A_2	A_3		A_4	Uncert.
283.0–338.0		8.596 08+1		−7.721 71	2.310 88			II

6.5.7.18. 4′-(Octyloxy)-4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid (47-086)

Name: 4′-(Octyloxy)-4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid

Formula: $C_{36}H_{46}O_5$
CAS-RN: 103376-72-3
Group No: 47-086

Experimental heat capacities (47.86.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997ASA/SOR		422.2–460.4	28	n/a	n/a	n/a	p	BSAO	1992SOR/KAJ

Parameters of regression polynomial (47.86.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	28	28	0.381	6.21−1	0.38	4.08−3	−1		
T/K		A_1		A_2		A_3		A_4	Uncert.
422.2–460.4		5.157 53+4		−3.438 75+4		7.665 09+3		−5.695 03+2	IV

6.5.7.19. 4′-[(1-Oxononyl)oxy]-4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid (47-087)

Name: 4′-[(1-Oxononyl)oxy]-4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester [1,1′-biphenyl]-4-carboxylic acid

Formula: $C_{37}H_{46}O_6$
CAS-RN: 135861-12-0
Group No: 47-087

Experimental heat capacities (47.87.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997ASA/SOR		422.7–449.6	17	n/a	n/a	n/a	p	BSAO	1992SOR/KAJ

Parameters of regression polynomial (47.87.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	17	17	0.058	9.11−2	0.06	5.25−3	1		
T/K		A_1		A_2		A_3		A_4	Uncert.
422.7–449.6		4.710 84+4		−3.176 95+4		7.165 27+3		−5.386 73+2	IV

6.6. Main group 5: compounds of carbon, hydrogen, and sulfur

6.6.3. Sub group 51: sulfides

6.6.3.1. Tetrakis(methylthia)methane (51-012)

Name:	Tetrakis(methylthia)methane
Formula:	$C_5H_{12}S$
CAS-RN:	6156-25-8
Group No:	51-012

Experimental heat capacities (51.12.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1943BAC/PER		338.6	1	n/a	99.75	melpt	p	BSIO	1943BAC/PER
1998SOR/KIM		339.4–357.2	11	n/a	99.93	melpt	p	BSAO	1992SOR/KAJ

Correlated heat capacities (51.12.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1998SOR/KIM	341.2–357.2	9	1.00	#	0.034	1.28−2	0.03	8.05−6	0

Parameters of regression polynomial (51.12.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	9	0.039	1.46−2	0.04	8.05−6	0
T/K		A_1		A_2	A_3	A_4	Uncert.
341.2–357.2		2.404 17+1		3.901 12			V

Deviation plot for Tetrakis(methylthia)methane (51-012) is given in Fig. 143.

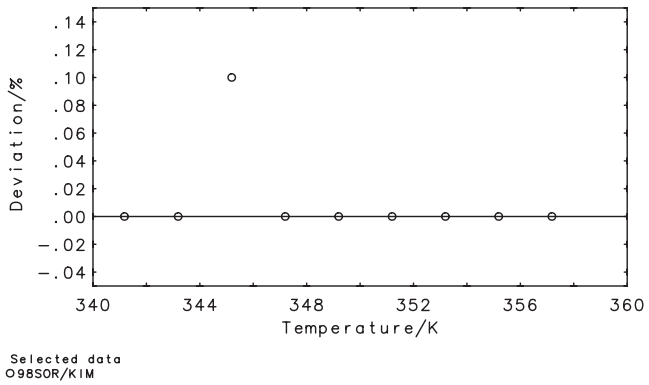

FIG. 143. Deviation plot for tetrakis(methylthia)methane (51-012).

6.6.3.2. 1,1′-Thiobis(cyclohexane) (51-030)

Name:	1,1′-Thiobis(cyclohexane)
Formula:	$C_{12}H_{22}S$
CAS-RN:	7133-46-2
Group No:	51-030

Experimental heat capacities (51.30.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference	
1997STE/CHI4	N	290.0–520.0	eqn		1.00	99.95	chrom	sat	BDHT	1989KNI/ARC
2004STE/CHI2		287.6–440.0	15		0.10	99.8	melpt	sat	BSAO	1988STE/ARC
2004STE/CHI2		460.0–520.0	4	S	1.00	99.8	melpt	sat	BDHT	1989KNI/ARC

Reference	Notes
1997STE/CHI4	original equation gives negative heat capacities; sign of second parameter was changed to positive

6.6.4. Sub group 52: thiols

None in this evaluation.

6.6.5. Sub group 53: heterocyclic sulfur compounds

6.6.5.1. 1,3,5-Trithiane (53-015)

Name:	1,3,5-Trithiane
Formula:	$C_3H_6S_3$
CAS-RN:	291-21-4
Group No:	53-015

Experimental heat capacities (53.15.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002VAN/VAN2		488.4–500.0	2	S	0.50	99.0	melpt	p	BDHT	2002VAN/VAN2

6.6.5.2. 2,3-Dihydrobenzo[*b*]thiophene (53-016)

Name:	2,3-Dihydrobenzo[b]thiophene
Formula:	C_8H_8S
CAS-RN:	4565-32-6
Group No:	53-016

Experimental heat capacities (53.16.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003STE/CHI		253.1–434.8	18		0.20	99.85	melpt	sat	BSAO	1988STE/ARC
2003STE/CHI		460.0–680.0	12	S	1.00	99.85	melpt	sat	BDHT	1989KNI/ARC

Correlated heat capacities (53.16.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2003STE/CHI	253.1–434.8	18	0.20	0.329	1.63−2	0.07	9.19−4	−2
2003STE/CHI	460.0–680.0	12	1.00	0.226	7.90−2	0.23	−3.36−2	−8

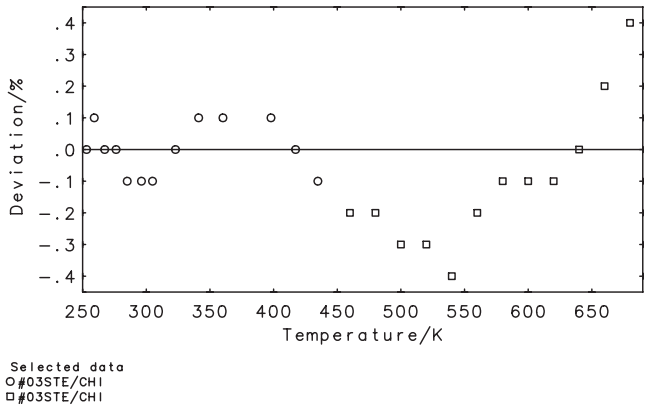

FIG. 144. Deviation plot for 2,3-dihydrobenzo[*b*]thiophene (53-016).

Parameters of regression polynomial (53.16.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−			
sat	30	30	0.314	5.53−2	0.16	−1.29−2	−10			
T/K			A_1		A_2		A_3		A_4	Uncert.
253.1–680.0			1.659 77+1		8.216 45−1		7.065 32−1		−4.927 11−2	III

Deviation plot for 2,3-Dihydrobenzo[*b*]thiophene (53-016) is given in Fig. 144.

6.6.5.3. 1,2,3,4-Tetrahydrodibenzothiophene (53-017)

Name:	1,2,3,4-Tetrahydrodibenzothiophene
Formula:	$C_{12}H_{12}S$
CAS-RN:	16587-33-0
Group No:	53-017

Experimental heat capacities (53.17.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004STE/CHI1		282.3–330.8	8		0.10	99.85	melpt	sat	BSAO	1988STE/ARC
2004STE/CHI1		440.0–600.0	9	S	1.00	99.85	melpt	sat	BDHT	1989KNI/ARC

Correlated heat capacities (53.17.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004STE/CHI1	282.3–330.8	8	0.10	0.405	1.31−2	0.04	−3.09−4	−1
2004STE/CHI1	440.0–600.0	9	1.00	0.283	1.32−1	0.28	2.89−2	3

Parameters of regression polynomial (53.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
sat	17	17	0.381	1.06−1	0.23	1.51−2	2		
T/K		A_1		A_2		A_3		A_4	Uncert.
282.3–600.0		1.492 77+1		5.452 14		1.208 87−1			II

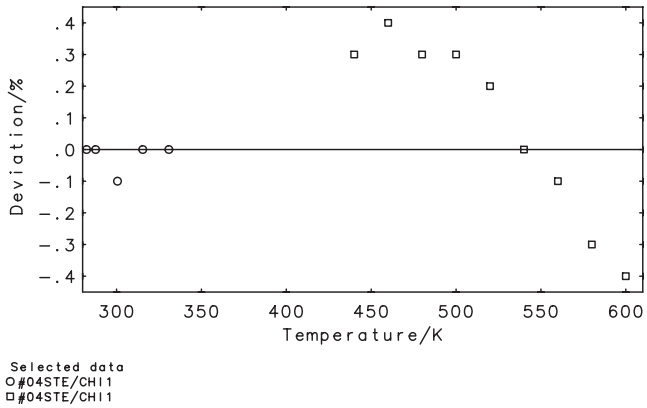

FIG. 145. Deviation plot for 1,2,3,4-tetrahydrodibenzothiophene (53-017).

Parameters of quasi-polynomial equation (53.17.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	17	17	0.261	4.21−2	0.09	−6.41−3	−5

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
282.3–600.0	825.00	2.164 28+1	8.665 85−1	1.580 65+1	5.580 18+1	3.270 78+1	7.601 66	II

Deviation plot for 1,2,3,4-Tetrahydrodibenzothiophene (53-017) is given in Fig. 145.

6.7. Main group 6: other organic compounds containing halogens, nitrogen, oxygen, and sulfur

6.7.3. Sub group 61: compounds of carbon, hydrogen, halogens, and oxygen

6.7.3.1. Trichloroacetaldehyde (61-003)

Name:	Trichloroacetaldehyde
Formula:	C_2HCl_3O
CAS-RN:	75-87-6
Group No:	61-003

Experimental heat capacities (61.3.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference	
1877BER	N	342.6	1		n/a	n/a	n/a	avg	DSIO	1879BER
1881VON		317.3–329.0	3	S	n/a	n/a	n/a	avg	DSIO	1881VON
1991VAS/LEB		135.0–330.0	12	S	0.20	99.92	chrom	*p*	BSAO	1976LEB/LIT

Reference	Notes
1877BER	average value in the temperature range 324−361 K

6.7.3.2. 2-Chlorophenol (61-037)

Name:	2-Chlorophenol
Formula:	C_6H_5ClO
CAS-RN:	95-57-8
Group No:	61-037

Experimental heat capacities (61.37.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference	
1916BRA		283.1–323.1	2		n/a	n/a	n/a	avg	DSTO	1916BRA
1937ELL		298.1–351.1	3	S	n/a	n/a	n/a	*p*	BSIO	1937ELL
2002LIP/SCH	N	293.1–353.1	7		0.50	99.97	chrom	*p*	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 2000ROH

6.7.3.3. 4-Chlorobenzoic acid (61-042)

Name:	4-Chlorobenzoic acid
Formula:	$C_7H_5ClO_2$
CAS-RN:	74-11-3
Group No:	61-042

Experimental heat capacities (61.42.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1926AND/LYN	N	512.8–538.2	2	n/a	n/a	n/a	*p*	DSIO	1926AND/LYN
2002TAN/SUN		514.9–579.3	11	0.40	99.935	melpt	sat	BSAO	1995TAN/SUN

Reference	Notes
1926AND/LYN	constant value calculated from temperature dependence of enthalpy by the authors

Correlated heat capacities (61.42.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002TAN/SUN	514.9–579.3	11	0.40	0.286	4.65−2	0.11	1.13−4	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1926AND/LYN	(2.18, 5.06, 2.18, 1)

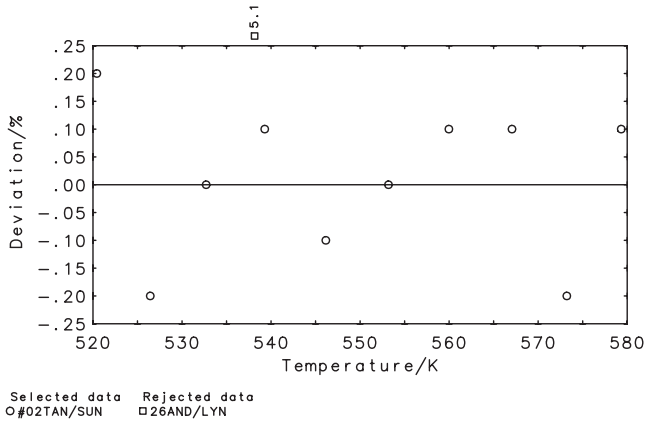

FIG. 146. Deviation plot for 4-chlorobenzoic acid (61-042).

Parameters of cubic spline polynomials (61.42.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	13	11	0.388	6.29−2	0.16	1.13−4	0

T/K	A_1	A_2	A_3	A_4	Uncert.
514.9–545.0	1.076 24+4	−6.116 06+3	1.160 40+3	−7.323 53+1	II
545.0–579.3	−1.969 72+4	1.065 07+4	−1.916 07+3	1.149 28+2	III

Deviation plot for 4–Chlorobenzoic acid (61–042) is given in Fig. 146.

6.7.3.4. 3-Chlorophenol (61-051)

Name:	3-Chlorophenol
Formula:	C_6H_5ClO
CAS-RN:	108-43-0
Group No:	61-051

Experimental heat capacities (61.51.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002LIP/SCH	N	313.1–353.1	5	0.50	99.97	chrom	p	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 2000ROH

6.7.3.5. 4-Chlorophenol (61-052)

Name:	4-Chlorophenol
Formula:	C_6H_5ClO
CAS-RN:	106-48-9
Group No:	61-052

Experimental heat capacities (61.52.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002LIP/SCH	N	323.1–353.1	4	0.50	99.81	chrom	p	BDCT	1983ROU/ROU

Reference	Notes
2002LIP/SCH	same data in 2000ROH

6.7.3.6. 1-Chloro-2-propanol (61-056)

Name:	1-Chloro-2-propanol
Formula:	C_3H_7ClO
CAS-RN:	127-00-4
Group No:	61-056

Experimental heat capacities (61.56.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI2		315.0–415.0	6	S	n/a	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (61.56.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	6	6	0.411	5.26−2	0.21	1.14−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
315.0–415.0	1.557 38+1	2.947 67			II

6.7.3.7. Heptafluorobutanoic acid (61-057)

Name:	Heptafluorobutanoic acid
Formula:	$C_4HF_7O_2$
CAS-RN:	375-22-4
Group No:	61-057

Experimental heat capacities (61.57.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI6		293.0–398.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (61.57.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	11	11	0.027	1.01−2	0.03	5.69−5	−1
sat	11	11	0.000	2.20−6	0.00	1.04−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
293.0–398.0	5.513 09	8.843 39			II
293.0–398.0	5.650 00	8.800 00			III

Parameters of quasipolynomial equation (61.57.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.006	2.38−3	0.01	1.91−7	−1

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
293.0–398.3	530.00	−1.286 98	1.015 25−2	5.272 97	4.719 28+1	−3.269 00	7.563 42−2	I

6.7.3.8. Tridecafluoroheptanoic acid (61-058)

Name:	Tridecafluoroheptanoic acid
Formula:	$C_7HF_{13}O_2$
CAS-RN:	375-85-9
Group No:	61-058

Experimental heat capacities (61.58.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002STE/CHI2		330.0–510.0	10	S	n/a	99.95	chrom	sat	BDHT	1989KNI/ARC

Parameters of regression polynomial (61.58.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.402	2.58−1	0.40	2.10−3	2
sat	10	10	0.774	2.43−1	0.39	1.13−3	0

T/K	A_1	A_2	A_3	A_4	Uncert.
330.0–510.0	1.679 37+1	1.131 81+1			III
330.0–510.0	1.766 06+1	1.108 27+1			III

Parameters of quasipolynomial equation (61.58.4)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.433	2.74−1	0.43	1.42−3	2

T/K	T_c/K	A_1	A_2	A_3	A_4	A_5	A_6	Uncert.
330.0–510.0	583.00	−3.45 662	8.232 38−2	8.287 51	9.336 83+1	−3.377 13+1	4.162 09	IV

6.7.3.9. 2,4-Dichlorobenzaldehyde (61-059)

Name:	2,4-Dichlorobenzaldehyde
Formula:	$C_7H_4Cl_2O$
CAS-RN:	874-42-0
Group No:	61-059

Experimental heat capacities (61.59.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004WAN/TAN2		350.1–371.5	18	0.20	99.21	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (61.59.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	18	18	0.393	2.01−2	0.08	2.83−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
350.1–371.5	1.246 88+1	3.591 46			II

6.7.3.10. 3,6-Dichloro-2-methoxybenzoic acid (61-060)

Name:	3,6-Dichloro-2-methoxybenzoic acid
Formula:	$C_8H_6O_3Cl_2$
CAS-RN:	1918-00-9
Group No:	61-060

Experimental heat capacities (61.60.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001DI/LI		391.5–401.6	6	0.50	99.31	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (61.60.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	0.193	4.07−2	0.10	5.28−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
391.5–401.6	−1.303 87	1.091 73+1			II

6.7.3.11. 1,2,3,4-Tetrachlorodibenzo[*b*,*e*][1,4]dioxin (61-061)

Name: 1,2,3,4-Tetrachlorodibenzo[*b*,*e*][1,4]dioxin

Formula: $C_{12}H_4Cl_4O_2$
CAS-RN: 30746-58-8
Group No: 61-061

Experimental heat capacities (61.61.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001LEB/SMI		458.7–490.0	5	S	1.50	n/a	n/a	p	BDHT	1985GUS/DAV

Parameters of regression polynomial (61.61.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.051	3.54−2	0.08	2.44−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
458.7–490.0	−7.167 57	1.149 38+1			IV

6.7.3.12. 4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4′-propyl-1,1′-biphenyl (61-062)

Name: 4-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3,5-difluoro-4′-propyl-1,1′-biphenyl

Formula: $C_{22}H_{15}F_7O$
CAS-RN: 303186-20-1
Group No: 61-062

Experimental heat capacities (61.62.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004ZOU/TAN		317.8–338.9	10	0.40	99.7	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (61.62.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.214	7.29−2	0.09	4.28−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
317.8–338.9	9.307 43+3	−8.387 25+3	2.534 59+3	−2.544 86+2	III

6.7.4. Sub group 62: compounds of carbon, hydrogen, nitrogen, and oxygen

6.7.4.1. Nitromethane (62-002)

Name:	Nitromethane
Formula:	CH_3NO_2
CAS-RN:	75-52-5
Group No:	62-002

Experimental heat capacities (62.2.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1907WAL		290.1	1		n/a	n/a	n/a	avg	DSIO	1907WAL
1925WIL	N	303.0–343.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1925WIL	N	288.0–343.0	eqn		n/a	n/a	n/a	*p*	BSAO	1924WIL/DAN
1947JON/GIA		249.8–297.1	11		n/a	99.7	melpt	*p*	BSIO	1937GIA/EGA
1950HOU/MAS2		313.1–363.1	6	S	0.40	99.8	estim	*p*	BSAO	1950SAG/HOU
1965ZIE	N	316.0–333.9	2		n/a	n/a	n/a	avg	DSIO	1958SWI/ZIE1
1969BER/WES		308.1–473.1	18	S	0.10	99.99	melpt	sat	BSAO	1968WES/WES
1999CER/TOV		288.1–308.1	4		n/a	99.	chrom	*p*	BDCT	1983ROU/ROU
2000CER/MIG	N	288.1–308.1	4		n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2000CER/MIG	N	288.1–308.1	4		n/a	n/a	n/a	*p*	BDCT	1983ROU/ROU
2001CER/TOV1		288.1–308.1	4		n/a	99.0	chrom	*p*	BDHT	1969PER/COM

Reference	Notes
1925WIL	sample was dried P_2O_5
1925WIL	sample was dried $CaCl_2$
1965ZIE	average values in the temperature ranges 294–374 and 294–338 K
2000CER/MIG	Scanning method
2000CER/MIG	Isothermal step method

6.7.4.2. *N*,*N*-Dimethylformamide (62-016)

Name:	*N*,*N*-Dimethylformamide
Formula:	C_3H_7NO
CAS-RN:	68-12-2
Group No:	62-016

Experimental heat capacities (62.16.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1961GEL		273.0–323.0	5	S	n/a	n/a	n/a	*p*	n/a	n/a
1970ANO		293.2–423.2	8	S	n/a	n/a	n/a	sat	n/a	n/a
1973MOS/NIK		212.6–298.1	4	S	n/a	99.5	melpt	*p*	BSAO	1966NIK/LEB
1974DEV/SOM	N	298.1	1		0.50	n/a	n/a	*p*	BSIO	1970LKB/COM
1976BON/CER		298.1	1		n/a	n/a	n/a	*p*	BSIO	1976BON/CER
1977BON/BED	N	298.1	1		0.10	n/a	n/a	*p*	BSIO	1976BON/CER
1977DEV/PER2		298.1	1		0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1977DEV/PER3		298.1	1		0.50	n/a	n/a	*p*	FSIT	1971PIC/LED
1977VYU		298.0	1		n/a	n/a	n/a	*p*	n/a	n/a
1978MAR/CIO1	N	298.1–429.1	2		n/a	n/a	n/a	*p*	DSIO	1971MAR/CIO
1979DEV/SOM		298.1	1		1.00	99.8	chrom	*p*	BSIO	1970LKB/COM
1982VOR/YAK		298.1	1		n/a	n/a	n/a	*p*	BSAO	1977VOR/PRI
1984ZEG/SOM2		298.1	1		0.30	99.5	chrom	*p*	FSIT	1971PIC/LED

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1986KOR/KUK		278.0–298.0	2	0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1987PIE		298.1	1	n/a	99.5	chrom	*p*	FSIT	1971PIC/LED
1989KUL/KRE		308.0	1	n/a	n/a	n/a	*p*	BSAO	1983KUK/KOR
1989PET/PES1		258.1–318.1	4	n/a	n/a	n/a	*p*	BSAO	1983KUK/KOR
1991GRO/ROU		298.1	1	n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1992KOL/KUL2	N	283.1–323.1	6	0.05	n/a	n/a	*p*	BSAO	1975VYU/ZVE
1992MIY/TAM2		298.1	1	n/a	99.9	chrom	*p*	FSIO	1985OGA
1993NAK/CHU		298.1	1	0.50	99.96	chrom	*p*	FSIO	1985OGA
1994CON/GIA1		298.1	1	n/a	n/a	n/a	*p*	FSIT	1988CON/GIA
1994PRA/RAJ		293.1–323.1	4	n/a	n/a	n/a	*p*	BDHT	1989PRA/RAJ
1995CON/GIA1		298.1	1	0.50	99.5	chrom	*p*	FSIT	1988CON/GIA

Reference	Notes
1974DEV/SOM	C_p values for *N*,*N*-dimethylformamide and formamide were interchanged
1977BON/BED	infrared spectrum indicated that sample was water-free
1978MAR/CIO1	constant value calculated from temperature dependence of enthalpy by the authors
1992KOL/KUL2	content of water is 0.01%–0.02% by the Karl Fischer method

6.7.4.3. 2-Amino-2-methyl-1-propanol (62-028)

Name:	2-Amino-2-methyl-1-propanol
Formula:	$C_4H_{11}NO$
CAS-RN:	124-68-5
Group No:	62-028

Experimental heat capacities (62.28.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1980ROU/ROB		298.1	1	0.30	n/a	n/a	*p*	FSIT	1971PIC/LED
1997MAH/HEP		322.8–397.8	4	n/a	99.0	chrom	*p*	BDCT	1991BAN/GAR
1999CHI/LIU		303.1–353.1	11	3.00	95.	anal	*p*	BDHT	1999CHI/LIU
2001CHE/LI		303.1–353.1	11	2.00	99.0	anal	*p*	BDHT	1999CHI/LIU
2002ZHA/HAW		303.1–368.1	14	2.00	n/a	n/a	*p*	BDHT	2002ZHA/HAW

Correlated heat capacities (62.28.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1980ROU/ROB	298.1	1	0.30		0.898	7.44−2	0.27	−7.44−2	−1
1997MAH/HEP	322.8–397.8	4	3.00	#	0.266	2.45−1	0.80	4.40−2	−2
1999CHI/LIU	303.1–353.1	11	3.00		0.410	3.65−1	1.23	1.35−1	3
2001CHE/LI	303.1–353.1	11	3.00	#	0.582	5.17−1	1.75	3.94−1	7
2002ZHA/HAW	303.1–368.1	14	3.00	#	0.644	5.80−1	1.93	1.46−1	0

Parameters of regression polynomial (62.28.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	41	41	0.566	4.90−1	1.64	1.94−1	7

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–397.8	2.938 31	8.297 35			V

Deviation plot for 2-Amino-2-methyl-1-propanol (62-028) is given in Fig. 147.

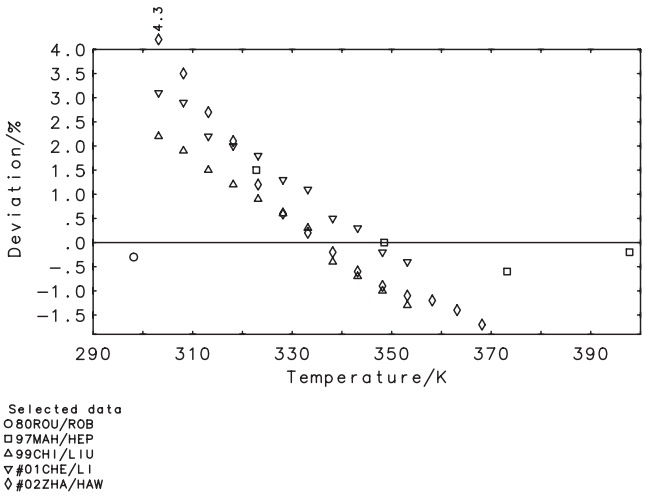

FIG. 147. Deviation plot for 2-amino-2-methyl-1-propanol (62-028).

6.7.4.4. Tetramethylurea (62-040)

Name:	Tetramethylurea
Formula:	$C_5H_{12}N_2O$
CAS-RN:	632-22-4
Group No:	62-040

Experimental heat capacities (62.40.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1988KOZ/KRA		320.0–425.0	eqn	2.00	n/a	n/a	p	BDHT	1992KAB/KOZ
1995KAB/KOZ1		274.5–302.0	15	2.00	n/a	n/a	sat	BDHT	1992KAB/KOZ

Correlated heat capacities (62.40.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1988KOZ/KRA	320.0–425.0	11	2.00	0.174	1.02−1	0.35	4.46−2	1
1995KAB/KOZ1	274.5–302.0	15	2.00	0.245	1.35−1	0.49	−3.09−2	1

Parameters of regression polynomial (62.40.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
C	26	26	0.232	1.30−1	0.46	1.08−3	2	
T/K		A_1		A_2	A_3		A_4	Uncert.
274.5–425.0		1.029 75+1		7.452 97	−5.259 05−1			V

Deviation plot for Tetramethylurea (62-040) is given in Fig. 148.

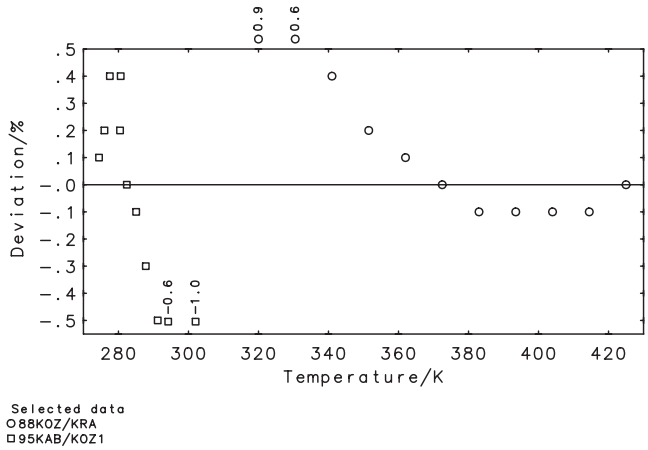

FIG. 148. Deviation plot for tetramethylurea (62-040).

6.7.4.5. Cyclohexanone oxime (62-052)

Name:	Cyclohexanone oxime
Formula:	$C_6H_{11}NO$
CAS-RN:	100-64-1
Group No:	62-052

Experimental heat capacities (62.52.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991KOZ/SHE	N	380.0–430.0	eqn	2.00	n/a	n/a	p	BDHT	1992KAB/KOZ
2002STE/CHI5		363.0–460.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1991KOZ/SHE	same equation in 1992KOZ/KAB

Correlated heat capacities (62.52.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2002STE/CHI5	363.0–460.2	10	1.00	0.000	0.00	0.00	0.00	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1991KOZ/SHE	(1.05, 2.98, −5.06−1, −2)

Parameters of regression polynomial (62.52.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	16	10	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
363.0–460.2	4.349 99	7.700 00			III

Deviation plot for Cyclohexanone oxime (62-052) is given in Fig. 149.

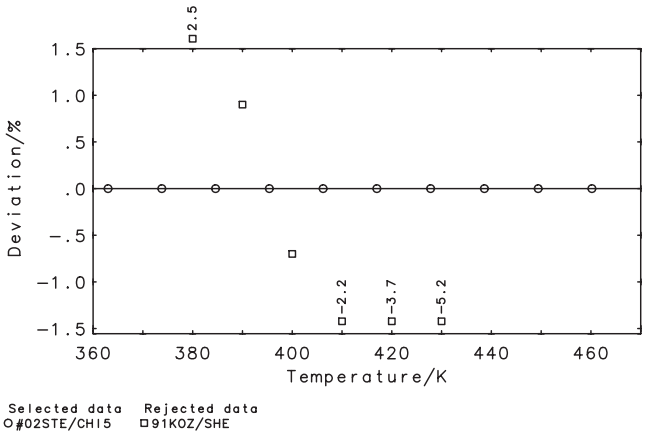

FIG. 149. Deviation plot for cyclohexanone oxime (62-052).

6.7.4.6. Hexahydro-2*H*-azepin-2-one (62-053)

Name:	Hexahydro-2*H*-azepin-2-one
Formula:	$C_6H_{11}NO$
CAS-RN:	105-60-2
Group No:	62-053

Experimental heat capacities (62.53.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1962KOL/PAU	N	345.0–375.0	7	S	n/a	99.95	melpt	*p*	BSAO	1956POP/KOL
1989KOZ/MAR		350.0–510.0	eqn		1.50	99.95	anal	*p*	BDHT	1992KAB/KOZ
1992KAB/KOZ	N	342.0–520.0	eqn		1.50	n/a	n/a	*p*	BDHT	1992KAB/KOZ
2002STE/CHI3		342.0–500.0	eqn		1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Reference	Notes
1962KOL/PAU	some data in 1959KOL/PAU and 1959PAU/KOL
1992KAB/KOZ	same equation in 1991KOZ/SHE

Correlated heat capacities (62.53.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1962KOL/PAU	345.0–375.0	7	1.50	#	0.489	2.24−1	0.73	1.83−1	5
1989KOZ/MAR	350.0–510.5	16	4.00	#	0.990	1.33	3.96	−1.16	−16
2002STE/CHI3	342.0–499.5	16	1.00		0.318	1.09−1	0.32	4.47−2	4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1992KAB/KOZ	(7.88, 19.47, 7.54, 17)

Parameters of regression polynomial (62.53.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	57	39	0.716	8.82−1	2.63	−4.24−1	−7
sat	57	39	0.716	8.82−1	2.63	−4.24−1	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
342.0–510.5	1.222 13+1	4.894 16			III
342.0–510.5	1.222 13+1	4.894 16			III

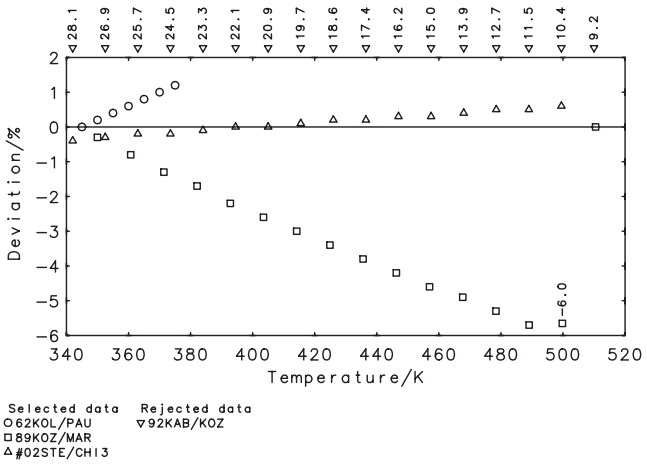

FIG. 150. Deviation plot for hexahydro-2*H*-azepin-2-one (62-053).

Deviation plot for Hexahydro-2*H*-azepin-2-one (62-053) is given in Fig. 150.

6.7.4.7. Tetraethyl urea (62-083)

Name:	Tetraethyl urea
Formula:	$C_9H_{20}N_2O$
CAS-RN:	1187-03-7
Group No:	62-083

Experimental heat capacities (62.83.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1990KOZ/SIM		290.0–370.0	eqn	2.00	n/a	n/a	*p*	BDHT	1992KAB/KOZ
1995KAB/KOZ1		243.3–304.8	15	2.00	99.9	chrom	sat	BDHT	1992KAB/KOZ

Correlated heat capacities (62.83.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1990KOZ/SIM	290.0–370.1	10	2.00	0.493	4.22−1	0.99	2.18−1	2
1995KAB/KOZ1	243.3–304.8	15	2.00	0.289	2.40−1	0.58	−1.37−1	−9

Parameters of regression polynomial (62.83.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	25	25	0.419	3.55−1	0.84	4.95−3	−7

T/K	A_1	A_2	A_3	A_4	Uncert.
243.3–370.1	1.502 85+2	−1.210 55+2	4.219 92+1	−4.620 18	III

Deviation plot for Tetraethyl urea (62-083) is given in Fig. 151.

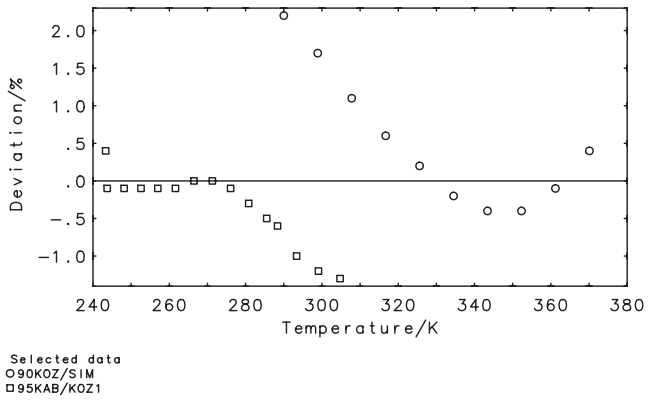

FIG. 151. Deviation plot for tetraethyl urea (62-083).

6.7.4.8. Tetrahydro-2*H*-1,3-oxazin-2-one (62-134)

Name:	Tetrahydro-2*H*-1,3-oxazin-2-one
Formula:	$C_4H_7NO_2$
CAS-RN:	5259-97-2
Group No:	62-134

Experimental heat capacities (62.134.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997LEB/SMI	N	400.3–446.2	22		2.50	n/a	n/a	p	BDHT	1969YAG
2002LEB/VER	N	354.0–450.0	3	S	2.50	n/a	n/a	p	BDHT	1985GUS/DAV

Reference	Notes
1997LEB/SMI	$C_p(T)$ anomaly at 350 to 400 K associated with melting of crystals (T_{mp}=354 K)
2002LEB/VER	smoothed data from 1997LEB/SMI

Correlated heat capacities (62.134.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1997LEB/SMI	400.3–446.2	22	2.50	0.153	1.04−1	0.38	−2.29−3	0
2002LEB/VER	354.0–450.0	3	2.50	0.068	4.14−2	0.17	2.32−2	1

Parameters of regression polynomial (62.134.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	25	25	0.152	1.03−1	0.38	7.68−4	1

T/K	A_1	A_2	A_3	A_4	Uncert.
354.0–450.0	4.741 36	5.386 83			V

Deviation plot for Tetrahydro-2*H*-1,3-oxazin-2-one (62-134) is given in Fig. 152.

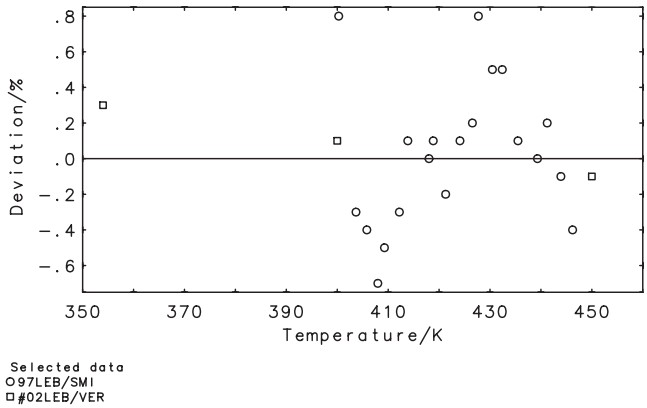

FIG. 152. Deviation plot for tetrahydro-2*H*-1,3-oxazin-2-one (62-134).

6.7.4.9. 2,2′-(Methylimino)bis(ethanol) (62-145)

Name:	2,2′-(Methylimino)bis(ethanol)
Formula:	$C_5H_{13}NO_2$
CAS-RN:	105-59-9
Group No:	62-145

Experimental heat capacities (62.145.1)

Reference	Note	*T*/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1994LEE		303.1–353.1	11	S	n/a	n/a	n/a	*p*	n/a	n/a
1997MAH/HEP		299.1–397.8	5		n/a	99.0	anal	*p*	BDCT	1991BAN/GAR
1999CHI/LIU		303.1–353.1	11		1.00	98.5	anal	*p*	BDHT	1999CHI/LIU
2001CHE/SHI		303.1–353.1	11		1.00	99.0	anal	*p*	BDHT	1999CHI/LIU
2002ZHA/HAW		278.1–368.1	19		2.00	99.01	chrom	*p*	BDHT	2002ZHA/HAW

Correlated heat capacities (62.145.2)

Reference	*T*/K	nPts	$\sigma_r C$/%		d_w	*d*/R	d_r/%	d_b/R	+/−
1994LEE	303.1–353.1	11	1.00	#	0.982	3.52−1	0.98	3.10−1	11
1997MAH/HEP	299.1–397.8	5	0.50	#	1.017	1.67−1	0.51	5.22−2	1
1999CHI/LIU	303.1–353.1	11	1.00		1.888	6.29−1	1.89	−6.20−1	−11
2001CHE/SHI	303.1–353.1	11	1.00		0.691	2.43−1	0.69	2.34−1	11
2002ZHA/HAW	278.1–368.1	19	2.00		0.248	1.63−1	0.50	4.44−2	1

Parameters of regression polynomial (62.145.3)

Type	nTot	nPts	s_w	*s*/R	s_r/%	s_b/R	+/−
p	57	57	1.057	3.57−1	1.05	4.84−3	13

T/K	A_1	A_2	A_3	A_4	Uncert.
278.1–397.8	9.873 85	7.475 41			V

Deviation plot for 2,2′-(Methylimino)bis(ethanol) (62-145) is given in Fig. 153.

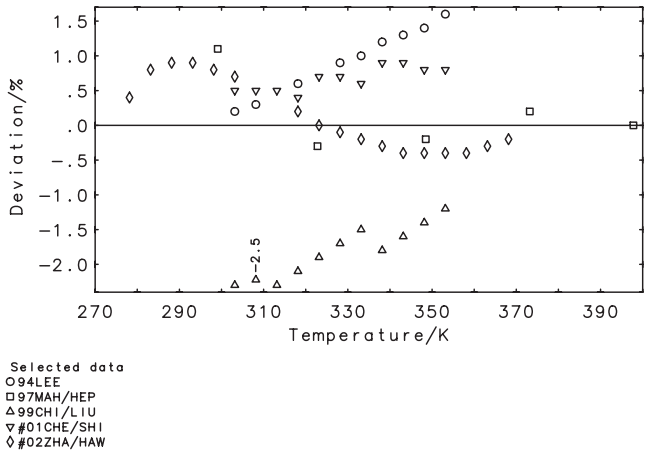

FIG. 153. Deviation plot for 2,2′-(methylimino)bis(ethanol) (62-145).

6.7.4.10. Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one (62-148)

Name:	Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one
Formula:	$C_6H_{11}NO_2$
CAS-RN:	54953-79-6
Group No:	62-148

Experimental heat capacities (62.148.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1996LEB/SMI		395.1–499.0	23		2.50	n/a	n/a	p	BDHT	1992KAB/KOZ
2002LEB/VER	N	390.0–500.0	4	S	2.50	n/a	n/a	p	BDHT	1985GUS/DAV

Reference	Notes
2002LEB/VER	smoothed data from 1997LEB/SMI

Correlated heat capacities (62.148.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
1996LEB/SMI	427.5–499.0	17	2.50	0.255	3.84−1	0.64	2.85−2	−3
2002LEB/VER	390.0–500.0	4	2.50	0.090	1.24−1	0.22	−9.84−2	−2

Parameters of regression polynomial (62.148.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	27	21	0.245	3.68−1	0.61	4.36−3	−5

T/K	A_1	A_2	A_3	A_4	Uncert.
390.0–500.0	4.994 80	1.172 42+1			V

Deviation plot for Tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one (62-148) is given in Fig. 154.

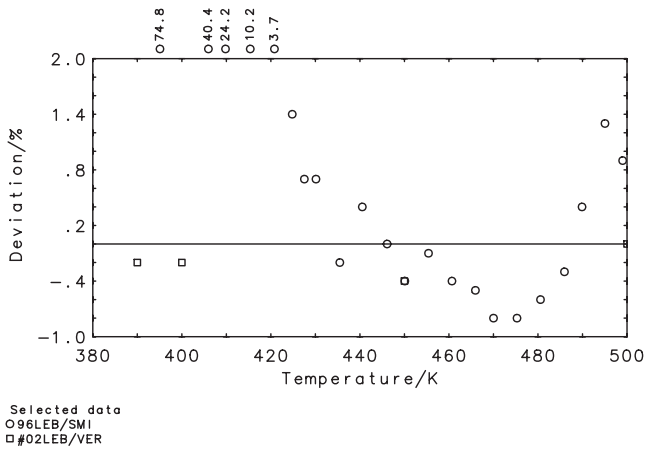

FIG. 154. Deviation plot for tetrahydro-5,5-dimethyl-2*H*-1,3-oxazin-2-one (62-148).

6.7.4.11. 2-(Diethylamino)ethanol (62-151)

Name:	2-(Diethylamino)ethanol
Formula:	$C_6H_{15}NO$
CAS-RN:	100-37-8
Group No:	62-151

Experimental heat capacities (62.151.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1997MAH/HEP		299.1–397.8	5	n/a	99.0	chrom	p	BDCT	1991BAN/GAR
2002STE/CHI6		293.0–458.0	eqn	1.00	99.95	chrom	sat	BDHT	1989KNI/ARC

Correlated heat capacities (62.151.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1997MAH/HEP	299.1–397.8	5	3.00	#	0.939	1.00	2.82	−9.89−1	−5
2002STE/CHI6	293.0–458.0	16	1.00		0.122	4.39−2	0.12	3.65−2	16

Parameters of regression polynomial (62.151.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	21	21	0.495	5.16−1	1.45	−2.08−1	11
sat	21	21	0.495	5.17−1	1.45	−2.08−1	11

T/K	A_1	A_2	A_3	A_4	Uncert.
293.0–458.0	1.894 72+1	5.274 27			II
293.0–458.0	1.894 74+1	5.274 19			II

Deviation plot for 2-(Diethylamino)ethanol (62-151) is given in Fig. 155.

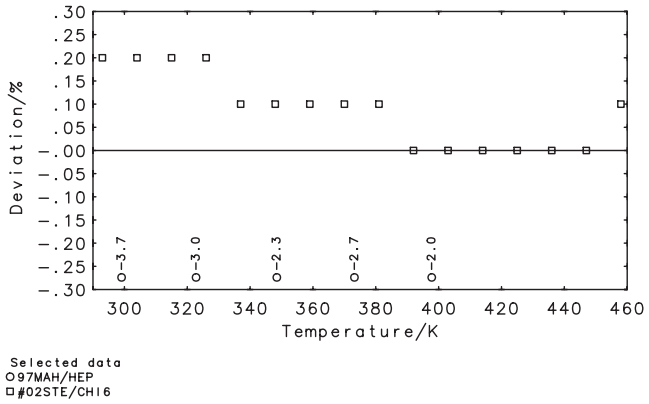

FIG. 155. Deviation plot for 2-(diethylamino)ethanol (62-151).

6.7.4.12. 2-Oxazolidinone (62-175)

Name:	2-Oxazolidinone
Formula:	$C_3H_5N_2O$
CAS-RN:	497-25-6
Group No:	62-175

Experimental heat capacities (62.175.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004SMI/MAR		363.1–373.5	13	1.50	n/a	n/a	p	BDHT	1992KAB/KOZ

Parameters of regression polynomial (62.175.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	13	13	1.113	2.97−1	1.67	8.43−3	−1
T/K		A_1		A_2	A_3	A_4	Uncert.
363.1–373.5		1.807 81+1		−1.813 33−2			V

6.7.4.13. Ethyl ester hydrazinecarboxylic acid (62-176)

Name:	Ethyl ester hydrazinecarboxylic acid
Formula:	$C_3H_8N_2O_2$
CAS-RN:	4114-31-2
Group No:	62-176

Experimental heat capacities (62.176.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001DI/SUN2		320.1–370.1	28	0.50	99.35	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.176.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	28	28	0.511	7.71−2	0.26	3.31−4	1

T/K	A_1	A_2	A_3	A_4	Uncert.
320.1–370.1	5.495 54+1	−3.676 45+1	8.654 36		III

6.7.4.14. 2,2′-Oxybis(ethanol) dinitrate (62-177)

Name:	2,2′-Oxybis(ethanol) dinitrate
Formula:	$C_4H_8N_2O_7$
CAS-RN:	693-21-0
Group No:	62-177

Experimental heat capacities (62.177.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000URY/KUP		276.5–320.0	4	S	0.30	99.2	melpt	p	BSAO	1976LEB/LIT

Parameters of regression polynomial (62.177.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
276.5–320.0	4.137 36+1				III

6.7.4.15. Ethyl ester 2-cyano-2-propenoic acid (62-178)

Name:	Ethyl ester 2-cyano-2-propenoic acid
Formula:	$C_6H_7NO_2$
CAS-RN:	7085-85-0
Group No:	62-178

Experimental heat capacities (62.178.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1991BYK/KIP		243.2–330.0	5	S	0.30	98.85	melpt	p	BSAO	1976LEB/LIT

Parameters of regression polynomial (62.178.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	5	5	0.421	3.36−2	0.13	4.58−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
243.2–330.0	2.118 53+1	2.049 19			II

6.7.4.16. 1,4-Diisocyanatobutane (62-179)

Name:	1,4-Diisocyanatobutane
Formula:	$C_6H_8N_2O_2$
CAS-RN:	4538-37-8
Group No:	62-179

Experimental heat capacities (62.179.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006SMI/KAN		236.4–358.7	59	0.20	99.54	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (62.179.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	59	59	0.425	2.29−2	0.09	3.70−5	−9

T/K	A_1	A_2	A_3	A_4	Uncert.
236.4–358.7	2.536 66+1	−1.351 87	6.447 06−1		II

6.7.4.17. 1-Ethyl-2-pyrrolidinone (62-180)

Name:	1-Ethyl-2-pyrrolidinone
Formula:	$C_6H_{11}NO$
CAS-RN:	2687-91-4
Group No:	62-180

Experimental heat capacities (62.180.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001BEC/GME		310.0–415.1	22	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF

Parameters of regression polynomial (62.180.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
sat	22	22	0.342	4.67−2	0.17	2.40−4	−5

T/K	A_1	A_2	A_3	A_4	Uncert.
310.0–415.1	1.054 00+1	4.550 72			IV

6.7.4.18. 2,4-Dinitrobenzaldehyde (62-181)

Name:	2,4-Dinitrobenzaldehyde
Formula:	$C_7H_4N_2O_5$
CAS-RN:	528-75-6
Group No:	62-181

Experimental heat capacities (62.181.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005WAN/TAN2		348.1–367.1	15	0.30	99.5	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.181.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	15	15	2.160	2.64−1	0.65	−6.13−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
348.1–367.1	5.368 79+4	4.519 81+4	−1.268 66+4	1.188 18+3	V

6.7.4.19. Phenyl-2-pyridinylmethanone (62-182)

Name:	Phenyl-2-pyridinylmethanone
Formula:	$C_{12}H_9NO$
CAS-RN:	91-02-1
Group No:	62-182

Experimental heat capacities (62.182.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006WAN/TAN		319.5–341.7	11	0.50	99.6	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.182.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	11	11	0.171	3.24−2	0.09	3.43−5	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
319.5–341.7		−7.268 41+1		5.927 61+1		−7.825 41		II

6.7.4.20. (1*R*,2*S*,5*R*)-5-Methyl-2-(1-methylethyl)cyclohexyl ester diazoacetic acid (62-183)

Name:	(1*R*,2*S*,5*R*)-5-Methyl-2-(1-methylethyl)cyclohexyl ester diazoacetic acid
Formula:	$C_{12}H_{20}N_2O_2$
CAS-RN:	63254-50-2
Group No:	62-183

Experimental heat capacities (62.183.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2000DI/TAN1		323.1–343.2	11	0.50	99.61	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.183.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	11	11	0.204	5.68−2	0.10	9.40−5	−2
T/K		A_1		A_2	A_3	A_4	Uncert.
323.1–343.2		4.992 31+1		1.690 14			III

6.7.4.21. 1′,3′-Dihydro-1′,3′,3′-trimethyl-6-nitrospiro[2*H*]-1-benzopyran-2,2′-[2*H*]indole (62-184)

Name:	1′,3′-Dihydro-1′,3′,3′-trimethyl-6-nitrospiro [2*H*]-1-benzopyran-2,2′-[2*H*] indole
Formula:	$C_{19}H_{18}N_2O_3$
CAS-RN:	1498-88-0
Group No:	62-184

Experimental heat capacities (62.184.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004KUL/MAR		459.2–472.4	7	1.50	99.0	chrom	p	BDHT	1985GUS/DAV

Parameters of regression polynomial (62.184.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	7	7	0.042	5.31−2	0.06	2.18−5	0

T/K	A_1	A_2	A_3	A_4	Uncert.
459.2–472.4	−6.757 51+2	3.093 20+2	−3.141 27+1		IV

6.7.4.22. 2,2,3,3-Tetramethylcyano(3-phenoxyphenyl)methyl ester cyclopropanecarboxylic acid (62-185)

Name: 2,2,3,3-Tetramethylcyano(3-phenoxyphenyl)methyl ester cyclopropanecarboxylic acid

Formula: $C_{22}H_{23}NO_3$
CAS-RN: 39515-41-8
Group No: 62-185

Experimental heat capacities (62.185.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001TAN/XUE	N	324.9–400.0	24	0.20	99.16	melpt	p	BSAO	1999TAN/ZHA

Reference	Notes
2001TAN/XUE	same data in 1999XUE/TAN

Parameters of cubic spline polynomials (62.185.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	24	24	1.452	2.25−1	0.29	1.04−3	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
324.9–360.0	3.395 41+3	−2.850 21+3	8.116 59+2	−7.662 97+1	IV
360.0–400.0	−7.007 43+2	5.632 54+2	−1.365 25+2	1.116 52+1	IV

6.7.4.23. Dodecanoic acid, comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1) (62-186)

Name: Dodecanoic acid, comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1) (62-186)

Formula: $C_{24}H_{37}N_3O_2$
CAS-RN: 218765-43-6
Group No: 62-186

Experimental heat capacities (62.186.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004SUN/LIU		323.5–339.3	10	0.50	99.43	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.186.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	10	10	0.199	1.03−1	0.10	1.25−4	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
323.5–339.3	−3.713 84+2	2.540 47+2	−3.349 23+1		II

6.7.4.24. Tetradecanoic acid comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1) (62-187)

Name:	Tetradecanoic acid comp. with 4,6-dimethyl-*N*-phenyl-2-pyrimidinamine (1:1) (62-187)
Formula:	$C_{26}H_{41}N_3O_2$
CAS-RN:	218765-45-8
Group No:	62-187

Experimental heat capacities (62.187.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004WAN/TAN3		323.2–360.5	40	0.50	98.99	melpt	*p*	BSAO	1995TAN/SUN

Parameters of regression polynomial (62.187.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	40	40	0.335	1.54−1	0.17	4.67−4	6

T/K	A_1	A_2	A_3	A_4	Uncert.
323.2–360.5	3.236 32+1	1.778 70+1			II

6.7.5. Sub group 63: compounds of carbon, hydrogen, oxygen, and sulfur

6.7.5.1. Sulfinylbis(methane) (63-001)

Name:	Sulfinylbis(methane)
Formula:	C_2H_6OS
CAS-RN:	67-68-5
Group No:	63-001

Experimental heat capacities (63.1.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1960KEN/LIN		298.1–343.1	2	n/a	n/a	n/a	*p*	BSIO	1957KEN
1962MUR/YAM	N	315.6	1	n/a	n/a	n/a	avg	n/a	n/a
1962SHE/NIN	N	288.1	1	n/a	n/a	n/a	*p*	n/a	n/a
1970CLE/WES		295.8–348.0	12	0.15	99.96	chrom	*p*	BSAO	1968WES/FUR
1978DEV/HEU		298.1	1	1.00	99.8	chrom	*p*	BSIO	1970LKB/COM
1979DEV/SOM		298.1	1	1.00	99.8	chrom	*p*	BSIO	1970LKB/COM
1986KOR/KUK		298.0	1	0.20	n/a	n/a	*p*	BSAO	1983KUK/KOR
1987LAN/CRI	N	298.1–353.1	3	n/a	n/a	n/a	*p*	FSIO	1987LAN/CRI
1988ROD/MAR	N	298.1	1	n/a	n/a	n/a	*p*	BSIO	1988ROD/MAR
1989BAR/KOO1		298.1	1	n/a	n/a	n/a	*p*	FSIT	1971PIC/LED
1991GRO/ROU		298.1	1	n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1992MIY/TAM1		298.1	1	n/a	99.6	chrom	*p*	FSIO	1985OGA

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1993BAS/VOL	N	298.1	1	n/a	99.5	chrom	*p*	DDCT	1971KON/SUU
1993CON/GIR1		298.0–356.0	eqn	5.00	n/a	n/a	sat	BDHT	1993CON/GIR1
1993GRO/ROU		298.1	1	n/a	99.5	anal	*p*	FSIT	1971PIC/LED
1993NAK/CHU		298.1	1	0.50	99.97	chrom	*p*	FSIO	1985OGA
1994GRO/ROU		298.1	1	n/a	99.0	anal	*p*	FSIT	1971PIC/LED
2001BEC/GME		310.0–415.1	22	0.50	99.95	chrom	sat	BDCT	2000BEC/AUF
2005FRA/BIG		298.1–318.1	3	n/a	99.9	chrom	*p*	BDHT	1995DIO/MAN

Reference	Notes
1962MUR/YAM	average value in the temperature range 298 – 333 K
1962SHE/NIN	very unrealable data below melting temperature
1987LAN/CRI	C_p at 298.15 K measured by Picker calorimeter (1971PIC/LED)
1988ROD/MAR	water contents is 0.0009% (Karl Fisher method)
1993BAS/VOL	content of water less than 0.05 mol % by the Karl Fischer method

Correlated heat capacities (63.1.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1970CLE/WES	295.8–348.0	12	0.15		0.619	1.74−2	0.09	−1.58−3	3
1987LAN/CRI	298.1–353.1	3	1.00	#	0.101	1.91−2	0.10	−3.43−3	1
1993BAS/VOL	298.1	1	1.00	#	0.130	2.39−2	0.13	−2.39−2	−1
1993CON/GIR1	298.0–356.1	8	5.00		0.662	6.42−1	3.31	6.37−1	8
2001BEC/GME	310.0–415.1	22	0.50		0.305	2.95−2	0.15	8.13−3	5

Rejected data: Reference (d/R, d_r, d_b/R, +/-)

1960KEN/LIN	(4.07−1, 2.23, −1.06−1, 0)	1962MUR/YAM	(4.58, 19.76, 4.58, 1)
1978DEV/HEU	(3.37−1, 1.80, 3.37−1, 1)	1979DEV/SOM	(3.37−1, 1.80, 3.37−1, 1)
1986KOR/KUK	(1.39−2, 0.08, 1.39−2, 1)	1988ROD/MAR	(6.46−2, 0.35, 6.46−2, 1)
1989BAR/KOO1	(5.79−1, 3.25, −5.79−1, −1)	1991GRO/ROU	(4.92−1, 2.74, −4.92−1, −1)
1992MIY/TAM1	(5.83−1, 3.27, −5.83−1, −1)	1993GRO/ROU	(4.46−1, 2.48, −4.46−1, −1)
1993NAK/CHU	(5.83−1, 3.27, −5.83−1, −1)	1994GRO/ROU	(4.74−1, 2.64, −4.74−1, −1)
2005FRA/BIG	(1.26, 7.28, −1.26, −3)		

Parameters of regression polynomial (63.1.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	63	46	0.493	2.81−1	1.45	1.13−1	16

T/K	A_1	A_2	A_3	A_4	Uncert.
295.8–415.1	4.869 97	1.085 21+1	−3.098 58	3.294 76−1	III

Deviation plot for Sulfinylbis(methane) (63-001) is given in Fig. 156.

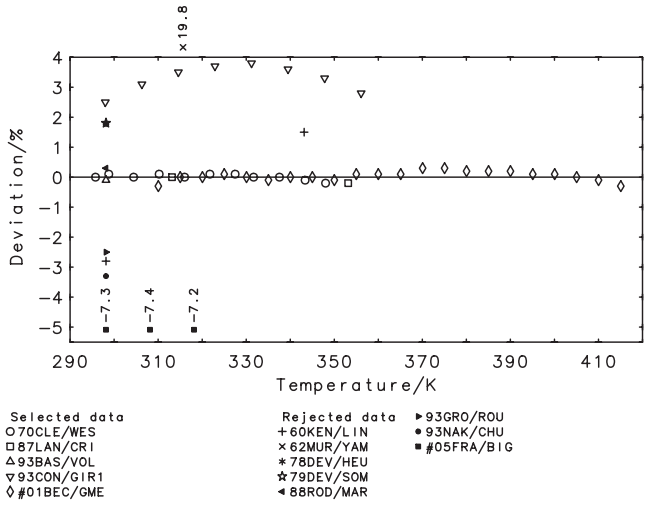

FIG. 156. Deviation plot for sulfinylbis(methane) (63-001)

6.7.5.2. (Methylsulfinyl)(methylthio)methane (63-009)

Name:	(Methylsulfinyl)(methylthio)methane
Formula:	$C_3H_8OS_2$
CAS-RN:	33577-16-1
Group No:	63-009

Experimental heat capacities (63.9.1)

Reference	Note	Temp.	C_p	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005MAS/NAG	N	298.15	1.77	n/a	99.95	anal	*p*	n/a	n/a

Reference	Notes
2005MAS/NAG	uknown DSC instrument used

6.7.6. Sub group 64: miscellaneous compounds

6.7.6.1. 1-Chloro-3-nitrobenzene (64-017)

Name:	1-Chloro-3-nitrobenzene
Formula:	$C_6H_4ClNO_2$
CAS-RN:	121-73-3
Group No:	64-017

Experimental heat capacities (64.17.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1894BRU	N	332.1	1	n/a	n/a	n/a	avg	DSIO	1894BRU
1908BOG/WIN	N	338.1	1	n/a	n/a	n/a	avg	DSIO	1908BOG/WIN
2007STR/RUZ		329.6-350.0	15	1.00	98.0	chrom	*p*	BDCT	2007STR/RUZ

Reference	Notes
1894BRU	average value in the temperature range 326–338 K
1908BOG/WIN	average value in the temperature range 318–358 K

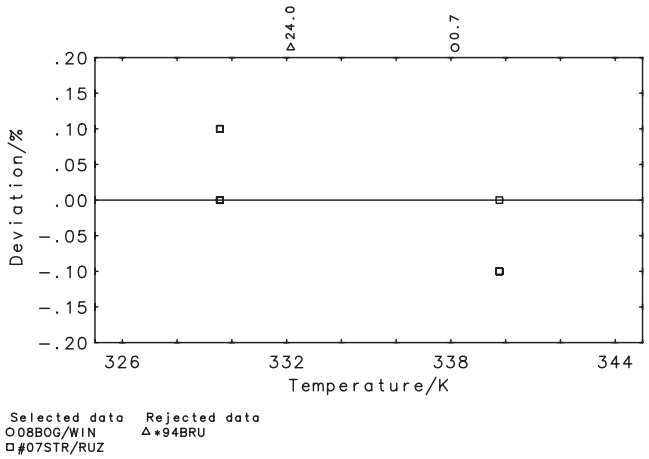

FIG. 157. Deviation plot for 1-chloro-3-nitrobenzene (64-017).

Correlated heat capacities (64.17.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1908BOG/WIN	338.1	1	3.00	#	0.222	1.77−1	0.67	1.77−1	1
2007STR/RUZ	329.6–350.0	15	1.00		0.072	1.89−2	0.07	−1.26−3	−4

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1894BRU	(8.29, 24.03, 8.29, 1)

Parameters of regression polynomial (64.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	17	16	0.095	5.12−2	0.19	9.87−3	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
329.6–350.0	1.604 75+1	3.056 68			III

Deviation plot for 1–Chloro—3–nitrobenzene (64–017) is given in Fig. 157.

6.7.6.2. 1-Chloro-2-nitrobenzene (64-042)

Name:	1-Chloro-2-nitrobenzene
Formula:	$C_6H_4ClNO_2$
CAS-RN:	88-73-3
Group No:	64-042

Experimental heat capacities (64.42.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2007STR/RUZ		319.4–350.0	12	1.00	99.0	chrom	p	BDCT	2007STR/RUZ

Parameters of regression polynomial (64.42.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.119	3.07−2	0.12	6.12−5	2

T/K	A_1	A_2	A_3	A_4	Uncert.
319.4–350.0	1.690 97+1	2.684 30			III

6.7.6.3. 2-Chlorobenzenamine (64-043)

Name:	2-Chlorobenzenamine
Formula:	C_6H_6ClN
CAS-RN:	95-51-2
Group No:	64-043

Experimental heat capacities (64.43.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2007STR/RUZ		268.3–350.0	31	1.00	99.5	chrom	p	BDCT	2007STR/RUZ

Parameters of regression polynomial (64.43.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	31	31	0.178	4.30−2	0.18	1.53−4	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
268.3–350.0	1.780 62+1	2.091 87			III

6.7.6.4. α-(Chloromethyl)-2-methyl-5-nitro-1*H*-imidazole-1-ethanol (64-044)

Name:	α-(Chloromethyl)-2-methyl-5-nitro-1*H*-imidazole-1-ethanol
Formula:	$C_7H_{10}ClN_3O_3$
CAS-RN:	16773-42-5
Group No:	64-044

Experimental heat capacities (64.44.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004WAN/TAN1		360.5-381.0	20	n/a	99.72	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (64.44.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	20	20	0.569	3.06−1	0.57	2.97−3	2

T/K	A_1	A_2	A_3	A_4	Uncert.
360.5−381.0	−4.068 61+2	2.339 04+2	−2.94883+1		III

6.7.6.5. 2-[(Chloromethyl)thio]benzothiazole (64-045)

Name: 2-[(Chloromethyl)thio]benzothiazole

Formula: $C_8H_6ClNS_2$
CAS-RN: 28908-00-1
Group No: 64-045

Experimental heat capacities (64.45.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005WAN/TAN1		316.6–348.8	10	0.50	99.21	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (64.45.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	10	10	0.203	4.08−2	0.10	6.18−5	1	
T/K		A_1		A_2		A_3	A_4	Uncert.
316.6–348.8		9.139 84+1		−3.800 19+1		6.824 81		II

6.7.6.6. 5,6-Dihydro-2-methyl-*N*-phenyl-1,4-oxathiin-3-carboxamide (64-046)

Name: 5,6-Dihydro-2-methyl-*N*–phenyl-1,4-oxathiin-3-carboxamide

Formula: $C_{12}H_{13}NO_2S$
CAS-RN: 5234-68-4
Group No: 64-046

Experimental heat capacities (64.46.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004WAN/TAN4		367.3–380.5	16	0.50	99.55	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (64.46.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	16	16	1.035	2.77−1	0.52	2.50−3	−2
T/K		A_1		A_2	A_3	A_4	Uncert.
367.3–380.5		1.949 52		1.376 28+1			IV

6.7.6.7. 1-[2-(2,4-Dichlorophenyl)pentyl-1*H*-1,2,4-triazole (64-047)

Name: 1-[2-(2,4-Dichlorophenyl)pentyl-1*H*-1,2,4-triazole

Formula: $C_{13}H_{15}Cl_2N_3$
CAS-RN: 66246-88-6
Group No: 64-047

Experimental heat capacities (64.47.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004SUN/SON		333.6–363.8	12	0.50	99.5	melpt	p	BSAO	1995TAN/SUN

Parameters of regression polynomial (64.47.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	12	12	0.501	1.49−1	0.25	5.58−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
333.6–363.8	−1.30287+2	9.482 37+1	−1.150 89+1		III

6.8. Main group 7: organic compounds containing other elements than halogens, nitrogen, oxygen, and sulfur

6.8.3. Sub group 71: organosilicon compounds

6.8.3.1. Hexamethylcyclotrisiloxane (71-015)

Name:	Hexamethylcyclotrisiloxane
Formula:	$C_6H_{18}O_3Si_3$
CAS-RN:	541-05-9
Group No:	71-015

Experimental heat capacities (71.15.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1977KUL/DZH2		335.2–350.0	3	S	n/a	n/a	n/a	p	BSAO	1954STR/ICK
2005PAL/ORA		339.9–404.9	16		n/a	99.98	chrom	p	BDHT	1973PER/COM

Correlated heat capacities (71.15.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
1977KUL/DZH2	335.2–350.0	3	3.00	#	0.632	9.03−1	1.89	−8.88−1	−3
2005PAL/ORA	339.9–404.9	16	1.00	#	0.079	3.92−2	0.08	1.93−2	5

Parameters of regression polynomial (71.15.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.276	3.81−1	0.80	−1.24−1	2

T/K	A_1	A_2	A_3	A_4	Uncert.
335.2–404.9	3.002 24+1	5.459 76			III

Deviation plot for Hexamethylcyclotrisiloxane (71-015) is given in Fig. 158.

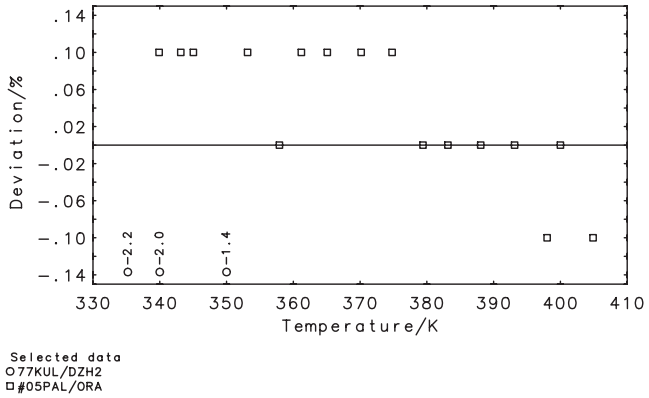

FIG. 158. Deviation plot for hexamethylcyclotrisiloxane (71-015).

6.8.3.2. Octamethylcyclotetrasiloxane (71-023)

Name:	Octamethylcyclotetrasiloxane
Formula:	$C_8H_{24}O_4Si_4$
CAS-RN:	556-67-2
Group No:	71-023

Experimental heat capacities (71.23.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1975MEK/KAR1		290.5–310.0	4	S	n/a	n/a	n/a	p	BSAO	1954STR/ICK
2005PAL/ORA		293.1–426.0	24		n/a	99.98	chrom	p	BDHT	1973PER/COM

Correlated heat capacities (71.23.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−	
2005PAL/ORA	293.1–426.0	24	1.00	#	0.099	6.45−2	0.10	1.26−4	1
Rejected data: Reference (d/R, d_r, d_b/R, +/−)									
1975MEK/KAR1	(2.10+1, 51.04, −2.10+1, −3)								

Parameters of regression polynomial (71.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	28	24	0.103	6.74−2	0.10	1.26−4	1
T/K		A_1		A_2	A_3	A_4	Uncert.
293.1–426.0		4.635 93+1		5.174 04			III

Deviation plot for Octamethylcyclotetrasiloxane (71-023) is given in Fig. 159.

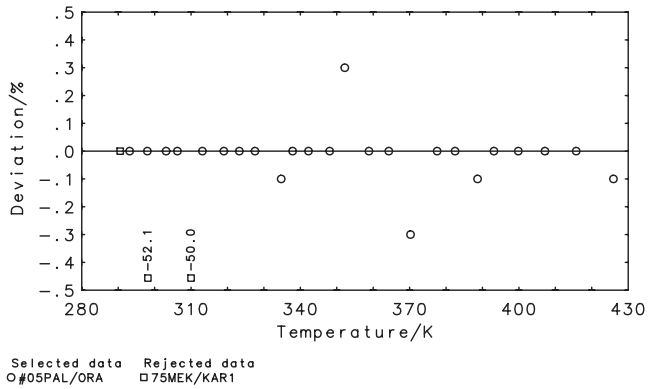

FIG. 159. Deviation plot for octamethylcyclotetrasiloxane (71-023).

6.8.3.3. Methyldi-2-propenylsilane (71-066)

Name:	Methyldi-2-propenylsilane
Formula:	$C_7H_{14}Si$
CAS-RN:	2043-08-5
Group No:	71-066

Experimental heat capacities (71.66.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001BYK/LEB		104.7–331.8	74	0.20	99.0	chrom	p	BSAO	1997VAR/DRU1

Parameters of cubic spline polynomials (71.66.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	74	74	1.087	5.62−2	0.22	2.30−4	2

T/K	A_1	A_2	A_3	A_4	Uncert.
104.7–140.0	−1.057 82+2	2.914 16+2	−2.174 71+2	5.407 53+1	III
140.0–180.0	6.543 48+1	−7.547 67+1	4.459 47+1	−8.321 41	IV
180.0–331.8	1.441 18+1	9.561 67	−2.648 83	4.273 99−1	IV

6.8.3.4. 1-(Triethylsilyl)aziridine (71-067)

Name:	1-(Triethylsilyl)aziridine
Formula:	$C_8H_{19}NSi$
CAS-RN:	15000-97-2
Group No:	71-067

Experimental heat capacities (71.67.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001SMI/LEB		184.9–348.1	88	0.20	99.22	melpt	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (71.67.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−			
p	88	87	0.823	5.56−2	0.16	1.75−4	13			
T/K		A_1		A_2		A_3		A_4		Uncert.
184.9–338.4		4.381 16+1		−1.536 37+1		6.120 22		−5.871 67−1		IV

6.8.3.5. Decamethylcyclopentasiloxane (71-068)

Name:	Decamethylcyclopentasiloxane
Formula:	$C_{10}H_{30}O_5Si_5$
CAS-RN:	541-02-6
Group No:	71-068

Experimental heat capacities (71.68.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005PAL/ORA		288.8–473.1	35	n/a	99.98	chrom	p	BDHT	1973PER/COM

Parameters of regression polynomial (71.68.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	35	35	0.063	5.09−2	0.06	4.23−5	4

T/K	A_1	A_2	A_3	A_4	Uncert.
288.8–473.1	6.050 69+1	5.555 24			III

6.8.3.6. Methyl ester 11-(1,1,3,3-tetramethyldisiloxanyl)undecanoic acid (71-069)

Name:	Methyl ester 11-(1,1,3,3-tetramethyldisiloxanyl)undecanoic acid
Formula:	$C_{16}H_{36}O_3Si_2$
CAS-RN:	349140-64-3
Group No:	71-069

Experimental heat capacities (71.69.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004RYA/LEB		233.3–340.0	5	S	0.20	n/a	n/a	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (71.69.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	5	5	0.378	5.28−2	0.08	3.81−5	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
233.3–340.0		3.523 65+1		1.826 85+1		−1.867 57		II

6.8.3.7. 4-Methoxy-4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]oxy]phenyl ester benzoic acid (71-070)

Name:	4-Methoxy-4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]oxy]phenyl ester benzoic acid
Formula:	$C_{29}H_{44}O_6Si_2$
CAS-RN:	349149-95-7
Group No:	71-070

Experimental heat capacities (71.70.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004RYA/LEB		334.0–350.0	2	S	0.20	n/a	n/a	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (71.70.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	2	2	0.000	0.00	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
334.0–350.0		−6.314 28+1		5.412 25+1				II

6.8.3.8. 4-Methoxyphenyl ester 4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]oxy]benzoic acid (71-071)

Name:	4-Methoxyphenyl ester 4-[[1-oxo-11-(1,1,3,3-tetramethyldisiloxanyl)undecyl]oxy]benzoic acid
Formula:	$C_{29}H_{44}O_6Si_2$
CAS-RN:	179108-75-9
Group No:	71-071

Experimental heat capacities (71.71.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004RYA/LEB		331.0350.0	2	S	0.20	n/a	n/a	p	BSAO	1997VAR/DRU1

Parameters of regression polynomial (71.71.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
331.0–350.0		1.238 80+2					II

6.8.4. Sub group 72: organic compounds containig phosphorus and boron

6.8.4.1. Hexamethylphosphorous triamide (72-023)

Name:	Hexamethylphosphorous triamide
Formula:	$C_6H_{18}N_3P$
CAS-RN:	1608-26-0
Group No:	72-023

Experimental heat capacities (72.23.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001SHE/KAR		226.7–296.2	25	0.20	99.59	melpt	p	BSAO	1985RAB/SHE

Parameters of regression polynomial (72.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	25	25	0.515	3.49−2	0.10	7.86−5	1

T/K	A_1	A_2	A_3	A_4	Uncert.
226.7–296.2	1.257 35+2	−1.109 34+2	4.227 45+1	−5.066 89	III

6.8.5. Sub group 73: organometallic compounds

6.8.5.1. Hexamethylarsenous triamide (73-055)

Name:	Hexamethylarsenous triamide
Formula:	$C_6H_{18}AsN_3$
CAS-RN:	6596-96-9
Group No:	73-055

Experimental heat capacities (73.55.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002SHE/KAR1		224.2–298.4	19	0.20	99.9	chrom	p	BSAO	1985RAB/SHE

Parameters of regression polynomial (73.55.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.975	7.24−2	0.19	2.18−4	−2

T/K	A_1	A_2	A_3	A_4	Uncert.
224.2–298.4	−2.092 50+1	5.985 32+1	−2.222 41+1	2.973 98	IV

6.8.5.2. Tripropylarsine (73-056)

Name:	Tripropylarsine
Formula:	$C_9H_{21}As$
CAS-RN:	5852-57-3
Group No:	73-056

Experimental heat capacities (73.56.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002SHE/KAR2		181.1–302.6	37	0.20	99.3	melpt	p	BSAO	1985RAB/SHE

Parameters of regression polynomial (73.56.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	37	37	0.756	5.53−2	0.15	1.48−4	1	
T/K		A_1		A_2		A_3	A_4	Uncert.
181.1–302.6		4.319 65+1		−1.547 11+1		7.278 91	−8.497 81−1	IV

6.8.5.3. Ethylferrocene (73-057)

Name:	Ethylferrocene
Formula:	$C_{12}H_{14}Fe$
CAS-RN:	1273-89-8
Group No:	73-057

Experimental heat capacities (73.57.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003KOZ/KAR	N	279.5–301.5	10	S	0.30	99.45	melpt	p	BSAO	1985RAB/SHE
Reference						Notes				
2003KOZ/KAR						smoothed values at 298.15 K in 2003KAR/KOZ				

Parameters of regression polynomial (73.57.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	10	10	0.242	2.87−2	0.07	3.32−5	−1	
T/K		A_1		A_2		A_3	A_4	Uncert.
279.5–301.5		−2.892 58+1		3.798 66+1		−4.949 08		II

6.8.5.4. [(Dimethylamino)methyl]ferrocene (73-058)

Name:	[(Dimethylamino)methyl]ferrocene
Formula:	$C_{13}H_{17}FeN$
CAS-RN:	1271-86-9
Group No:	73-058

Experimental heat capacities (73.58.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002KAR/SHE	N	283.0–295.6	4	S	0.30	97.59	melpt	p	BSAO	1985RAB/SHE
Reference						Notes				
2002KAR/SHE						extrapolated value at 298.15 K in 2003KAR/KOZ				

Parameters of regression polynomial (73.58.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	4	4	0.292	3.73−2	0.09	3.05−5	−1

T/K	A_1	A_2	A_3	A_4	Uncert.
283.0–295.6	1.349 89+1	1.021 83+1			II

6.8.5.5. Butylferrocene (73-059)

Name:	Butylferrocene
Formula:	$C_{14}H_8Fe$
CAS-RN:	31904-29-7
Group No:	73-059

Experimental heat capacities (73.59.1)

Reference	Note	T/K	nPts		Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2002KOZ/KAR	N	283.1–297.1	6	S	0.30	98.35	melpt	p	BSAO	1985RAB/SHE

Reference	Notes
2002KOZ/KAR	extrapolated value at 298.15 K in 2003KAR/KOZ

Parameters of regression polynomial (73.59.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	6	6	0.324	4.15−2	0.10	5.40−5	2

T/K	A_1	A_2	A_3	A_4	Uncert.
283.1–297.1	1.767 37+1	8.747 41			II

6.8.6. Sub group 74: salts of organic acids

6.8.6.1. Potassium salt hexanoic acid (74-032)

Name:	Potassium salt hexanoic acid
Formula:	$C_6H_{11}KO_2$
CAS-RN:	19455-00-6
Group No:	74-032

Experimental heat capacities (74.32.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2001NGE/MAL		549.2–600.2	17	n/a	99.9	melpt	p	BDHT	2001NGE/MAL

Parameters of regression polynomial (74.32.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	17	14	0.397	2.52−1	0.40	1.56−3	2

T/K	A_1	A_2	A_3	A_4	Uncert.
560.2–600.2	2.136 10+2	−5.844 29+1	5.595 11		V

6.8.7. Sub group 75: ionic liquids

6.8.7.1. 1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-001)

Name: 1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate

Formula: $C_6H_{11}BF_4N_2$
CAS-RN: 143314-16-3
Group No: 75-001

Experimental heat capacities (75.1.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
1998MUT/WIL		283.1–403.1	12	n/a	n/a	n/a	*p*	BDHT	1998MUT/WIL
2005WAL/STE		283.1–358.1	16	0.15	n/a	n/a	*p*	BDCT	2000ERN/CHO

Correlated heat capacities (75.1.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2005WAL/STE	283.1–358.1	16	0.15	0.037	2.11−3	0.01	1.19−6	0

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

1998MUT/WIL	(7.21, 23.60, −7.16, −7)

Parameters of regression polynomial (75.1.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	28	16	0.041	2.34−3	0.01	1.19−6	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
283.1–358.1		3.393 54+1		−1.847 33		9.708 87−1		I

Deviation plot for 1-Ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-001) is given in Fig. 160.

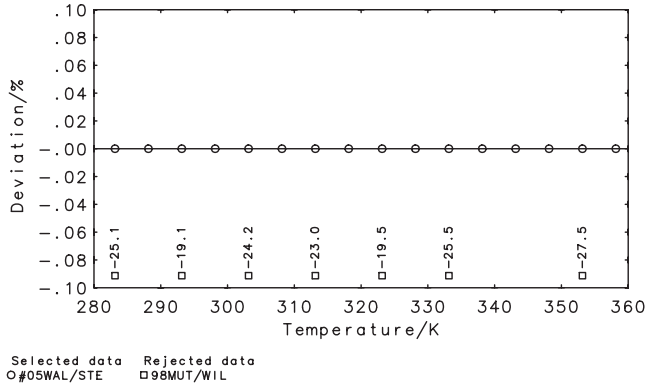

FIG. 160. Deviation plot for 1-ethyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-001).

6.8.7.2. 1-Ethyl-3-methyl-1*H*-imidazolium hexafluorophosphate (75-002)

Name: 1-Ethyl-3-methyl-1*H*-imidazolium hexafluorophosphate

Formula: $C_6H_{11}F_6N_2P$
CAS-RN: 155371-19-0
Group No: 75-002

Experimental heat capacities (75.2.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003HOL/REI		353.1–453.1	11	n/a	n/a	n/a	*p*	BDHT	1998MUT/WIL

Parameters of regression polynomial (75.2.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	11	11	0.268	1.03−1	0.27	3.27−4	1
T/K		A_1		A_2	A_3	A_4	Uncert.
353.1–453.1		1.031 18+1		6.931 09			IV

6.8.7.3. 1-Ethyl-3-methylimidazolium trifluoromethansulfonate (75-003)

Name: 1-Ethyl-3-methylimidazolium trifluoromethansulfonate

Formula: $C_7H_{11}F_3N_2O_3S$
CAS-RN: 145022-44-2
Group No: 75-003

Experimental heat capacities (75.3.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	*p*	BDHT	2004KIM/SHI
2006DIE/GME		313.1–423.1	23	n/a	n/a	n/a	*p*	BDCT	2000BEC/AUF

Correlated heat capacities (75.3.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.117	2.85−1	0.59	2.32−1	37
2006DIE/GME	313.1–423.1	23	5.00	#	0.195	4.63−1	0.98	−3.99−1	-21

Parameters of regression polynomial (75.3.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	64	64	0.153	3.65−1	0.76	5.42−3	16
T/K		A_1		A_2	A_3	A_4	Uncert.
313.1–425.1		3.250 52+1		4.355 40			IV

Deviation plot for 1-Ethyl-3-methylimidazolium trifluoromethansulfonate (75-003) is given in Fig. 161.

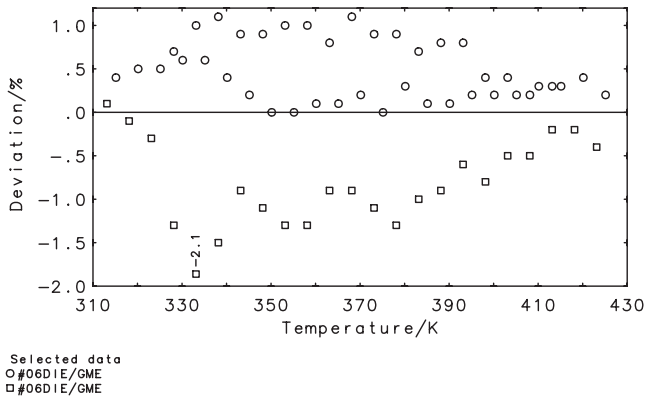

FIG. 161. Deviation plot for 1-ethyl-3-methylimidazolium trifluoromethansulfonate (75-003).

6.8.7.4. *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-propanaminium bromide (75-004)

Name: *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-propanaminium bromide

Formula: $C_7H_{18}BrNO$
CAS-RN: 13186-62-4
Group No: 75-004

Experimental heat capacities (75.4.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005DOM/BOG	N	382.5–430.0	48	n/a	n/a	n/a	*p*	BDCT	1989BRE/LIC

Reference	Notes
2005DOM/BOG	data in supporting Information

Parameters of regression polynomial (75.4.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	48	48	0.229	1.05−1	0.23	4.82−4	5
T/K		A_1		A_2	A_3	A_4	Uncert.
382.5–430.0		2.373 24+1		5.432 13			III

6.8.7.5. 1-Ethyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-005)

Name: 1-Ethyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide

Formula: $C_8H_{11}F_6N_3O_4S_2$
CAS-RN: 174899-82-2
Group No: 75-005

Experimental heat capacities (75.5.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO
2005WAL/STE		283.1–358.1	16	0.15	n/a	n/a	*p*	BDCT	2000ERN/CHO

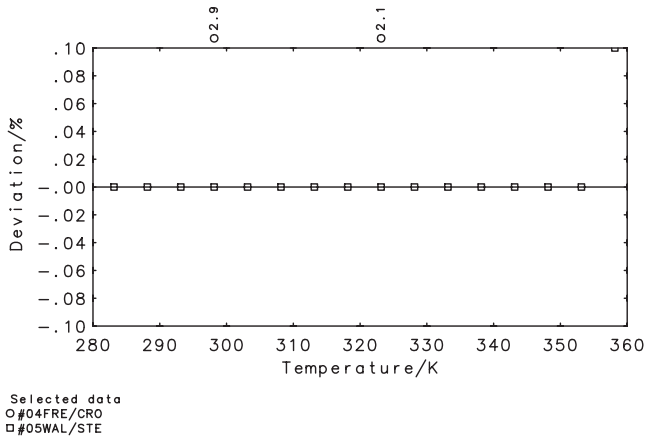

FIG. 162. Deviation plot for 1-ethyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-005).

Correlated heat capacities (75.5.2)

2004FRE/CRO	298.1–323.1	2	4.00	0.630	1.60	2.52	1.58	2
2005WAL/STE	283.1–358.1	16	0.15	0.202	1.90−2	0.03	−2.45−4	−3

Parameters of regression polynomial (75.5.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	18	18	0.301	5.65−1	0.89	1.75−1	−1
T/K		A_1		A_2	A_3	A_4	Uncert.
283.1–58.1		4.421 1+1		5.711 0			III

Deviation plot for 1-Ethyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-005) is given in Fig. 162.

6.8.7.6. 1-Butyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-006)

Name:	1-Butyl-3-methyl-1*H*-imidazolium tetrafluoroborate
Formula:	$C_8H_{15}BF_4N_2$
CAS-RN:	174501-65-6
Group No:	75-006

Experimental heat capacities (75.6.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO
2004KIM/SHI		298.2–320.2	10	2.00	n/a	n/a	*p*	BDHT	2004KIM/SHI
2004REB/NAJ		278.1–333.1	12	n/a	98.0	anal	*p*	BDHT	1969PER/COM
2005WAL/STE		283.1–358.1	16	0.15	n/a	n/a	*p*	BDCT	2000ERN/CHO

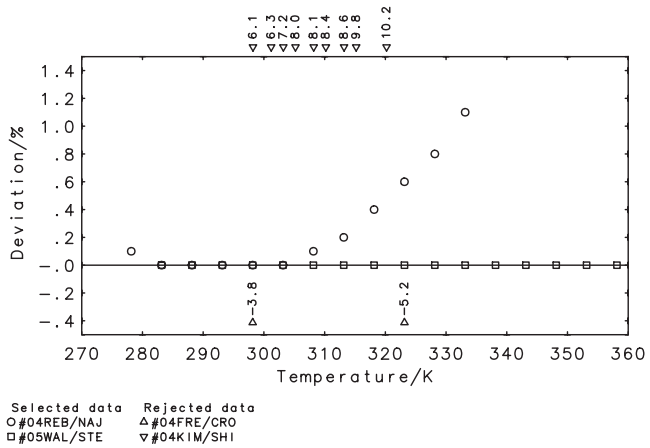

FIG. 163. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-006).

Correlated heat capacities (75.6.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2004REB/NAJ	278.1–333.1	12	1.00	#	0.453	2.09−1	0.45	1.23−1	5
2005WAL/STE	283.1–358.1	16	0.15		0.181	1.22−2	0.03	−2.04−3	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2004FRE/CRO	(1.96, 4.58, −1.93, −2)	2004KIM/SHI	(4.10, 8.39, 4.03, 10)

Parameters of regression polynomial (75.6.3).

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	40	28	0.339	1.42−1	0.31	5.17−2	3
T/K		A_1		A_2	A_3	A_4	Uncert.
278.1–358.1		2.677 75+1		5.736 33			II

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-006) is given in Fig. 163.

6.8.7.7. 1-Butyl-3-methyl-1*H*-imidazolium bromide (75-007)

Name:	1-Butyl-3-methyl-1*H*-imidazolium bromide
Formula:	$C_8H_{15}BrN_2$
CAS-RN:	85100-77-2
Group No:	75-007

Experimental heat capacities (75.7.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO
2004KIM/SHI		298.2–323.2	11	2.00	n/a	n/a	p	BDHT	2004KIM/SHI

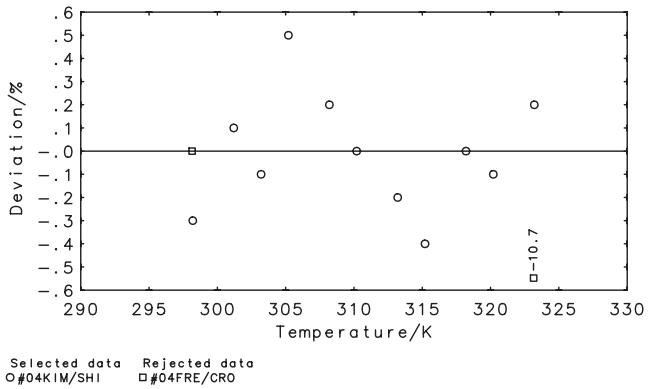

FIG. 164. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium bromide (75-007).

Correlated heat capacities (75.7.2)

Reference	T/K	nPts	$\sigma_r C$/%	d_w	d/R	d_r/%	d_b/R	+/−
2004KIM/SHI	298.2–323.2	11	2.00	0.123	9.56−2	0.25	4.42−4	1
Rejected data: Reference (d/R, d_r, d_b/R, +/−)								
2004FRE/CRO	(4.18, 10.74, −4.18, −1)							

Parameters of regression polynomial (75.7.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	13	11	0.135	1.06−1	0.27	4.42−4	1
T/K		A_1		A_2	A_3	A_4	Uncert.
298.2–323.2		−5.279 98+1		2.967 62+1			IV

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium bromide (75-007) is given in Fig. 164.

6.8.7.8. 1-Butyl-3-methyl-1*H*-imidazolium chloride (75-008)

Name:	1-Butyl-3-methyl-1*H*-imidazolium chloride
Formula:	$C_8H_{15}ClN_2$
CAS-RN:	79917-90-1
Group No:	75-008

Experimental heat capacities (75.8.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003HOL/REI		343.1–453.1	12	n/a	n/a	n/a	p	BDHT	1998MUT/WIL
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Correlated heat capacities (75.8.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2003HOL/REI	343.1–453.1	12	1.00	#	0.121	5.10−2	0.12	4.83−5	3

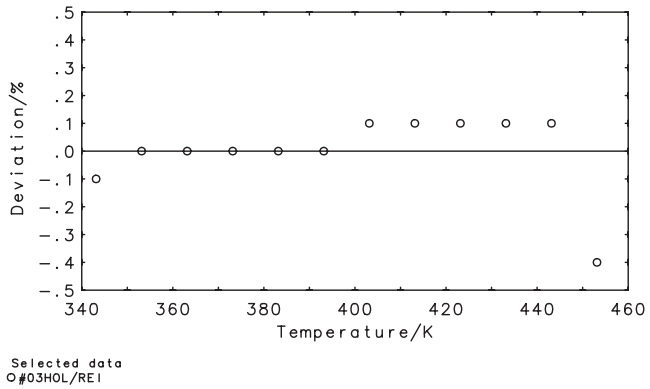

FIG. 165. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium chloride (75-008).

Parameters of regression polynomial (75.8.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	14	12	0.133	5.59−2	0.13	4.83−5	3
T/K		A_1		A_2	A_3	A_4	Uncert.
343.1–453.1		1.457 12+1		6.229 28			III

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium chloride (75-008) is given in Fig. 165.

6.8.7.9. 1-Butyl-3-methyl-1*H*-imidazolium hexafluorophosphate (75-009)

Name:	1-Butyl-3-methyl-1*H*-imidazolium hexafluorophosphate
Formula:	$C_8H_{15}F_6N_2P$
CAS-RN:	174501-64-5
Group No:	75-009

Experimental heat capacities (75.9.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003HOL/REI		303.1–453.1	16	n/a	n/a	n/a	*p*	BDHT	1998MUT/WIL
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO
2004KAB/BLO		285.3–305.3	13	n/a	n/a	n/a	sat	BDHT	1992KAB/KOZ
2004KAB/BLO		412.0–550.0	eqn	0.40	99.56	melpt	*p*	BSAO	1993DIK/KAB

Correlated heat capacities (75.9.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2004FRE/CRO	298.1–323.1	2	4.00		1.016	1.97	4.06	−1.90	−2
2004KAB/BLO	285.3–305.3	13	1.00	#	0.152	7.43−2	0.15	1.03−2	1
2004KAB/BLO	412.0–549.8	14	0.40		0.020	4.90−3	0.01	1.47−3	−2

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2003HOL/REI	(8.98, 20.19, −8.92, −16)

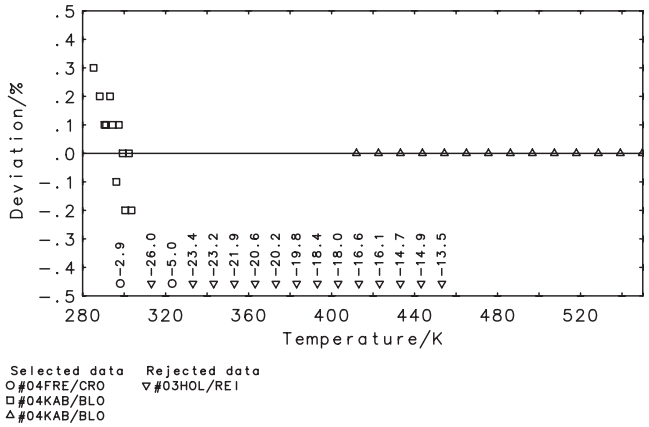

FIG. 166. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium hexafluorophosphate (75-009).

Parameters of regression polynomial (75.9.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
C	45	29	0.302	5.49−1	1.13	−1.26−1	−3

T/K	A_1	A_2	A_3	A_4	Uncert.
285.3–549.8	1.419 51+1	1.530 41+1	−1.196 81		IV

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium hexafluorophosphate (75-009) is given in Fig. 166.

6.8.7.10. *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-butanaminium bromide (75-010)

Name: *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-butanaminium bromide

Formula: $C_8H_{20}BrNO$
CAS-RN: 28508-15-8
Group No: 75-010

Experimental heat capacities (75.10.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005DOM/BOG	N	409.7–438.3	19	n/a	n/a	n/a	p	BDCT	1989BRE/LIC

Reference	Notes
2005DOM/BOG	data in supporting information

Parameters of regression polynomial (75.10.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	19	19	0.244	1.16−1	0.24	5.08−4	−4

T/K	A_1	A_2	A_3	A_4	Uncert.
409.7–438.3	8.042 33	9.290 95			III

6.8.7.11. 2,3-Dimethyl-1-ethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (75-011)

Name: 2,3-Dimethyl-1-ethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide

Formula: $C_9H_{13}F_6N_3O_4S_2$
CAS-RN: 174899-90-2
Group No: 75-011

Experimental heat capacities (75.11.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		309.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.11.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
309.1–323.1		4.305 74+1		5.240 42			VI

6.8.7.12. 1-Butyl-3-methyl-1*H*-imidazolium trifluoromethanesulfonate (75-012)

Name: 1-Butyl-3-methyl-1*H*-imidazolium trifluoromethanesulfonate

Formula: $C_9H_{15}F_3N_2O_3S$
CAS-RN: 174899-66-2
Group No: 75-012

Experimental heat capacities (75.12.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	*p*	BDHT	2004KIM/SHI
2006DIE/GME		313.2–423.1	23	n/a	n/a	n/a	*p*	BDCT	2000BEC/AUF

Correlated heat capacities (75.12.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.297	8.45−1	1.48	5.54−3	5
2006DIE/GME	313.2–423.1	23	5.00	#	0.094	2.56−1	0.47	3.77−2	9

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2004FRE/CRO	(2.92, 5.74, −2.92, −1)

Parameters of regression polynomial (75.12.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	66	64	0.248	7.05−1	1.24	1.71−2	14
T/K		A_1		A_2	A_3	A_4	Uncert.
313.2–425.1		3.506 02+1		5.801 14			III

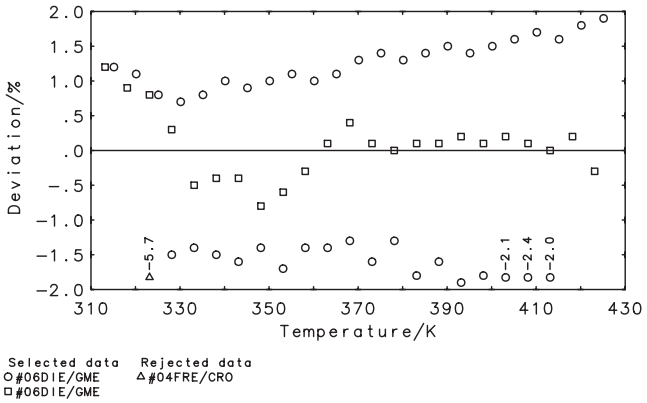

FIG. 167. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium trifluoromethanesulfonate (75-012).

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium trifluoromethanesulfonate (75-012) is given in Fig. 167.

6.8.7.13. 1-Butyl-2,3-dimethyl-1*H*-imidazolium tetrafluoroborate (75-013)

Name: 1-Butyl-2,3-dimethyl-1*H*-imidazolium tetrafluoroborate

Formula: $C_9H_{17}BF_4N_2$
CAS-RN: 402846-78-0
Group No: 75-013

Experimental heat capacities (75.13.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		330.1–372.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.13.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
330.1–372.1	1.564 09+1	8.934 50			VI

6.8.7.14. 1-Butyl-2,3-dimethyl-1*H*-imidazolium hexafluorophsophate (75-014)

Name: 1-Butyl-2,3-dimethyl-1*H*-imidazolium hexafluorophsophate

Formula: $C_9H_{17}F_6N_2P$
CAS-RN: 227617-70-1
Group No: 75-014

Experimental heat capacities (75.14.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.14.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–323.1	2.991 73+1	7.456 89			VI

6.8.7.15. 1-Butyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-015)

Name:	1-Butyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{10}H_{15}F_6N_3O_4S_2$
CAS-RN:	174899-83-3
Group No:	75-015

Experimental heat capacities (75.15.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003HOL/REI		293.1–453.1	17	n/a	n/a	n/a	*p*	BDHT	1998MUT/WIL
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	*p*	BDHT	2004FRE/CRO

Correlated heat capacities (75.15.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2003HOL/REI	293.1–453.1	17	1.00	#	0.460	2.89−1	0.46	2.82−3	−3
Rejected data: Reference (d/R, d_r, d_b/R, +/−)									
2004FRE/CRO	(1.06+1, 16.42, 1.06+1, 2)								

Parameters of regression polynomial (75.15.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−		
p	19	17	0.507	3.19−1	0.51	2.82−3	−3		
T/K		A_1		A_2		A_3	A_4	Uncert.	
293.1–453.1		−9.015 55−1		2.283 63+1		−1.620 86		III	

Deviation plot for 1-Butyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-015) is given in Fig. 168.

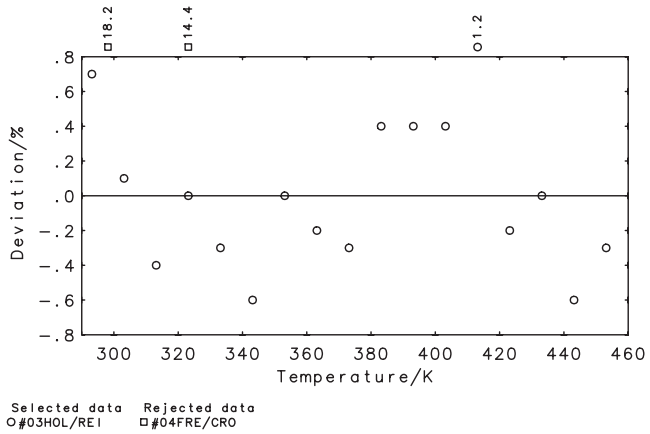

FIG. 168. Deviation plot for 1-butyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-015).

6.8.7.16. 2,3-Dimethyl-1-propyl-1*H*-imidazolium bis(trifluoromethylsulfonyl)imide (75-016)

Name: 2,3-Dimethyl-1-propyl-1*H*-imidazolium bis(trifluoromethylsulfonyl)imide

Formula: $C_{10}H_{15}F_6N_3O_4S_2$
CAS-RN: 169051-76-7
Group No: 75-016

Experimental heat capacities (75.16.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.16.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–323.1	6.066 65+1	2.020 60			VI

6.8.7.17. 1-Butyl-3-methyl-1*H*-imidazolium dicyanamide (75-017)

Name: 1-Butyl-3-methyl-1*H*-imidazolium dicyanamide

Formula: $C_{10}H_{15}N_5$
CAS-RN: 448245-52-1
Group No: 75-017

Experimental heat capacities (75.17.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.17.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–323.1	3.610 57+1	2.597 88			VI

6.8.7.18. 1-Butyl-3-methylpyridinium tetrafluoroborate (75-018)

Name: 1-Butyl-3-methylpyridinium tetrafluoroborate

Formula: $C_{10}H_{16}BF_4N$
CAS-RN: 597581-48-1
Group No: 75-018

Experimental heat capacities (75.18.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0-323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.18.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	2.577 19+1	7.697 42			VI

6.8.7.19. 1-Ethyl-3-methylpyridinium ethyl sulfate (75-019)

Name:	1-Ethyl-3-methylpyridinium ethyl sulfate
Formula:	$C_{10}H_{17}NO_4S$
CAS-RN:	872672-50-9
Group No:	75-019

Experimental heat capacities (75.19.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	*p*	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.19.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	2.814 85+1	6.254 17			VI

6.8.7.20. 1-Methyl-1-propylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-020)

Name:	1-Methyl-1-propylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{10}H_{18}F_6N_2O_4S_2$
CAS-RN:	223437-05-6
Group No:	75-020

Experimental heat capacities (75.20.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005WAL/STE		283.1–358.1	16	0.15	n/a	n/a	*p*	BDCT	2000ERN/CHO

Parameters of regression polynomial (75.20.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	16	16	0.108	1.11−2	0.02	8.58−6	0

T/K	A_1	A_2	A_3	A_4	Uncert.
283.1–358.1	4.284 21+1	7.979 41			III

6.8.7.21. 1-Hexyl-3-methyl-1*H*-imidazolium tetrafluoroborate (75-021)

Name: 1-Hexyl-3-methyl-1*H*-imidazolium tetrafluoroborate

Formula: $C_{10}H_{19}BF_4N_2$
CAS-RN: 244193-50-8
Group No: 75-021

Experimental heat capacities (75.21.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.21.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	2.566 13+1	8.178 50			VI

6.8.7.22. 1-Hexyl-3-methyl-1*H*-imidazolium bromide (75-022)

Name: 1-Hexyl-3-methyl-1*H*-imidazolium bromide

Formula: $C_{10}H_{19}BrN_2$
CAS-RN: 85100-78-3
Group No: 75-022

Experimental heat capacities (75.22.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.22.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	2.273 63+1	6.254 15			VI

6.8.7.23. 1-Hexyl-3-methyl-1*H*-imidazolium hexafluorophosphate (75-023)

Name: 1-Hexyl-3-methyl-1*H*-imidazolium hexafluorophosphate

Formula: $C_{10}H_{19}F_6N_2P$
CAS-RN: 304680-35-1
Group No: 75-023

Experimental heat capacities (75.23.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2003HOL/REI		303.1–453.1	16	n/a	n/a	n/a	p	BDHT	1998MUT/WIL

Parameters of regression polynomial (75.23.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	16	16	0.212	1.22−1	0.21	4.36−4	−1
T/K		A_1		A_2	A_3	A_4	Uncert.
303.1–453.1		1.958 40+1		1.035 04+1			II

6.8.7.24. *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-hexanaminium bromide (75-024)

Name: *N*-(2-Hydroxyethyl)-*N*,*N*-dimethyl-1-hexanaminium bromide

Formula: $C_{10}H_{24}BrNO$
CAS-RN: 219787-58-3
Group No: 75-024

Experimental heat capacities (75.24.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005DOM/BOG	N	386.4–403.4	13	n/a	n/a	n/a	p	BDCT	1989BRE/LIC

Reference	Notes
2005DOM/BOG	data in supporting information

Parameters of regression polynomial (75.24.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	13	13	0.084	4.75−2	0.08	6.87−5	1
T/K		A_1		A_2	A_3	A_4	Uncert.
386.4–403.4		2.897 08+1		6.976 81			III

6.8.7.25. 1-Butyl-pyridinium bis(trifluoromethylsulfonyl)imid (75-025)

Name: 1-Butyl-pyridinium bis(trifluoromethylsulfonyl)imid

Formula: $C_{11}H_{14}F_6N_2O_4S_2$
CAS-RN: 187863-42-9
Group No: 75-025

Experimental heat capacities (75.25.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		328.1–425.1	39	5.00	n/a	n/a	p	BDHT	2004KIM/SHI
2006DIE/GME		323.2–423.1	21	n/a	n/a	n/a	p	BDHT	2004KIM/SHI

Correlated heat capacities (75.25.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	328.1–425.1	39	5.00		0.250	9.32−1	1.25	3.53−1	3
2006DIE/GME	323.2–423.1	21	1.00	#	0.275	2.05−1	0.27	−2.35−2	−3

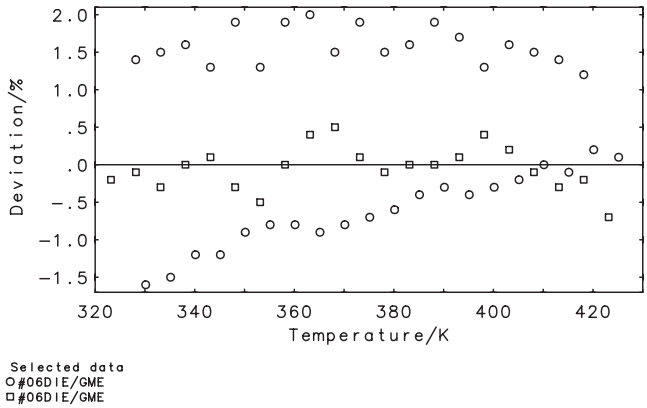

FIG. 169. Deviation plot for 1-butyl-pyridinium bis(trifluoromethylsulfonyl)imid (75-025).

Parameters of regression polynomial (75.25.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	60	60	0.263	7.74−1	1.04	2.21−1	0
T/K		A_1		A_2	A_3	A_4	Uncert.
323.2–425.1		5.332 56+1		5.568 77			IV

Deviation plot for 1-Butyl-pyridinium bis(trifluoromethylsulfonyl)imid (75-025) is given in Fig. 169.

6.8.7.26. *N*-Ethyl-4-4(*N′*,*N′*-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imid (75-026)

Name:	*N*-Ethyl-4–4(*N′*,*N′*-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imid

Formula: $C_{11}H_{15}F_6N_3O_4S_2$
CAS-RN: 900797-77-5
Group No: 75-026

Experimental heat capacities (75.26.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	p	BDHT	2004KIM/SHI
2006DIE/GME		313.1–423.2	23	n/a	n/a	n/a	p	BDCT	2000BEC/AUF

Correlated heat capacities (75.26.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.570	2.08	2.85	−1.44	−20
2006DIE/GME	313.1–423.2	23	1.00	#	0.622	4.69-1	0.62	1.17−1	7

Parameters of regression polynomial (75.26.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	64	64	0.598	1.72	2.35	−8.79−1	−13
T/K		A_1		A_2	A_3	A_4	Uncert.
313.1–425.1		5.948 99+1		4.483 14			IV

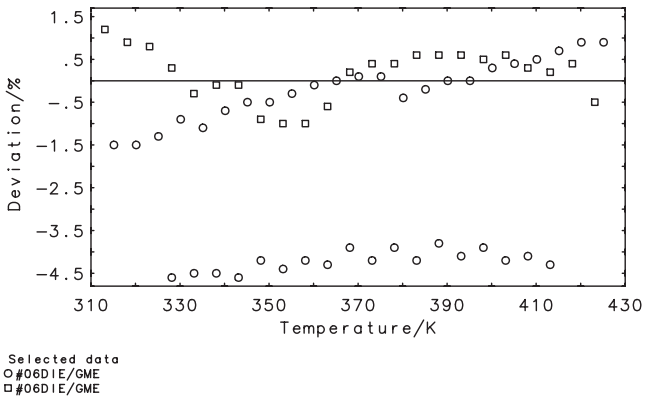

FIG. 170. Deviation plot for *N*-ethyl-4-4(*N*′,*N*′-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imid (75-026).

Deviation plot for *N*-Ethyl-4-4(*N*′,*N*′-dimethylammonium)pyridinium bis(trifluoromethylsulfonyl)imid (75-026) is given in Fig. 170.

6.8.7.27. 1-Hexyl-3-methylimidazolium trifluoromethanesulfonate (75-027)

Name: 1-Hexyl-3-methylimidazolium trifluoromethanesulfonate

Formula: $C_{11}H_{19}F_3N_2O_3S$
CAS-RN: 460345-16-8
Group No: 75-027

Experimental heat capacities (75.27.1)

Reference	Note	*T*/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	*p*	BDHT	2004KIM/SHI
2006DIE/GME		313.1–423.2	23	n/a	n/a	n/a	*p*	BDCT	2000BEC/AUF

Correlated heat capacities (75.27.2)

Reference	*T*/K	nPts	$\sigma_r C$/%		d_w	*d*/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.301	1.01	1.51	1.98−1	5
2006DIE/GME	313.1–423.2	23	1.00	#	0.185	1.22−1	0.18	−1.15−2	2

Parameters of regression polynomial (75.27.3)

Type	nTot	nPts	s_w	*s*/R	s_r/%	s_b/R	+/−
p	64	64	0.270	8.25−1	1.23	1.23−1	7

T/K	A_1	A_2	A_3	A_4	Uncert.
313.1–425.1	4.326 63+1	6.110 85			IV

Deviation plot for 1-Hexyl-3-methylimidazolium trifluoromethanesulfonate (75-027) is given in Fig. 171.

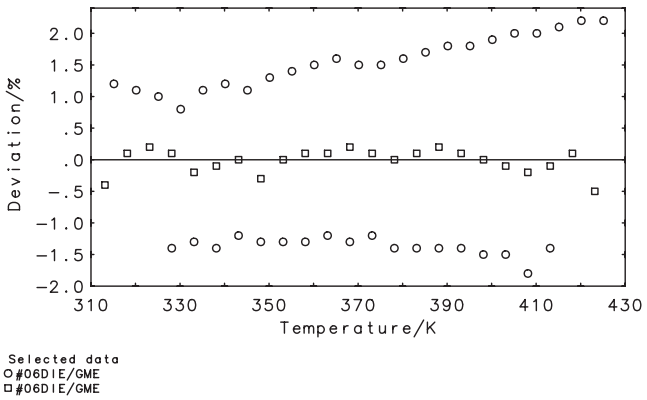

FIG. 171. Deviation plot for 1-hexyl-3-methylimidazolium trifluoromethanesulfonate (75-027).

6.8.7.28. 1-Methyl-3-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-028)

Name: 1-Methyl-3-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide

Formula: $C_{12}H_{10}F_{15}N_3O_4S_2$
CAS-RN: 872672-61-2
Group No: 75-028

Experimental heat capacities (75.28.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.28.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	2	2	0.000	0.00	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.0–323.0		4.848 90+1		1.298 94+1				VI

6.8.7.29. 1-Butyl-3-methyl-1*H*-imidazolium tris[(trifluoromethyl)sulfonyl]methane (75-029)

Name: 1-Butyl-3-methyl-1*H*-imidazolium tris[(trifluoromethyl)sulfonyl-]methane

Formula: $C_{12}H_{15}F_9N_2O_6S_2$
CAS-RN: 731774-32-6
Group No: 75-029

Experimental heat capacities (75.29.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2004FRE/CRO		298.1–323.1	2	4.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.29.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.1–323.1	6.603 56+1	9.429 32			VI

6.8.7.30. 1-Butyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-030)

Name:	1-Butyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{12}H_{16}F_6N_2O_4S_2$
CAS-RN:	344790-86-9
Group No:	75-030

Experimental heat capacities (75.30.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	*p*	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.30.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	4.757 01+1	9.140 69			VI

6.8.7.31. 1-Hexyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-031)

Name:	1-Hexyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{12}H_{19}F_6N_3O_4S_2$
CAS-RN:	382150-50-7
Group No:	75-031

Experimental heat capacities (75.31.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	*p*	BDHT	2004FRE/CRO
2006DIE/GME		320.1–425.1	41	5.00	n/a	n/a	*p*	BDHT	2004KIM/SHI
2006DIE/GME		318.2–418.1	21	n/a	n/a	n/a	*p*	BDCT	2000BEC/AUF

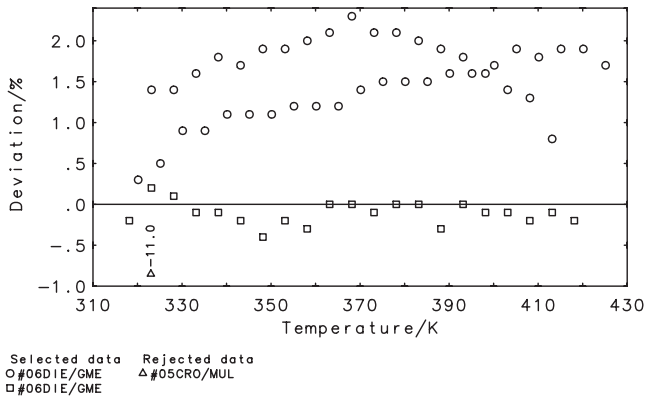

FIG. 172. Deviation plot for 1-hexyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-031).

Correlated heat capacities (75.31.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	320.1–425.1	41	5.00		0.319	1.36	1.59	1.30	41
2006DIE/GME	318.2–418.1	21	1.00	#	0.180	1.48−1	0.18	−9.78−2	−15

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2005CRO/MUL	(8.02, 11.04, −8.02, −1)

Parameters of regression polynomial (75.31.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	64	62	0.287	1.13	1.33	8.28−1	26

T/K	A_1	A_2	A_3	A_4	Uncert.
318.2–425.1	1.002 92+2	−1.565 52+1	2.965 33		IV

Deviation plot for 1-Hexyl-3-methyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-031) is given in Fig. 172.

6.8.7.32. 3-(Ethoxycarbonyl)-1-ethylpyridinium ethyl sulfate (75-032)

Name:	3-(Ethoxycarbonyl)-1-ethylpyridinium ethyl sulfate
Formula:	$C_{12}H_{19}NO_5S$
CAS-RN:	872672-51-0
Group No:	75-032

Experimental heat capacities (75.32.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.32.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	3.732 77+1	8.178 50			VI

6.8.7.33. 1-Hexyl-3-methylpyridinium bromide (75-033)

Name:	1-Hexyl-3-methylpyridinium bromide
Formula:	$C_{12}H_{20}BrN$
CAS-RN:	67021-56-1
Group No:	75-033

Experimental heat capacities (75.33.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.33.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
298.0–323.0		1.974 87+1		7.216 32			VI

6.8.7.34. 1-Methyl-3-octyl-1*H*-imidazolium tetrafluoroborate (75-034)

Name:	1-Methyl-3-octyl-1*H*-imidazolium tetrafluoroborate
Formula:	$C_{12}H_{23}BF_4N_2$
CAS-RN:	244193-52-0
Group No:	75-034

Experimental heat capacities (75.34.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.34.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
298.0–323.0		3.218 48+1		9.621 78			VI

6.8.7.35. 1-Methyl-3-octylimidazolium bromide (75-035)

Name:	1-Methyl-3-octylimidazolium bromide
Formula:	$C_{12}H_{23}BrN_2$
CAS-RN:	61545-99-1
Group No:	75-035

Experimental heat capacities (75.35.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.35.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
298.0–323.0		2.420 84+1		7.697 42			VI

6.8.7.36. 1-Hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-036)

Name:	1-Hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{13}H_{18}F_6N_2O_4S_2$
CAS-RN:	460983-97-5
Group No:	75-036

Experimental heat capacities (75.36.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.36.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0
T/K		A_1		A_2	A_3	A_4	Uncert.
298.0–323.0		4.493 37+1		9.621 77			VI

6.8.7.37. 1-Butyl-4-dimethylaminopyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-037)

Name:	1-Butyl-4-dimethylaminopyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{13}H_{19}F_6N_3O_4S_2$
CAS-RN:	900797-79-7
Group No:	75-037

Experimental heat capacities (75.37.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		315.1–425.1	40	5.00	n/a	n/a	p	BDHT	2004KIM/SHI
2006DIE/GME		313.1–423.1	24	n/a	n/a	n/a	p	BDCT	2000BEC/AUF

Correlated heat capacities (75.37.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	40	5.00		0.184	7.74−1	0.92	2.76−1	19
2006DIE/GME	313.1–423.1	24	1.00	#	0.268	2.25-1	0.27	−1.63−2	−2

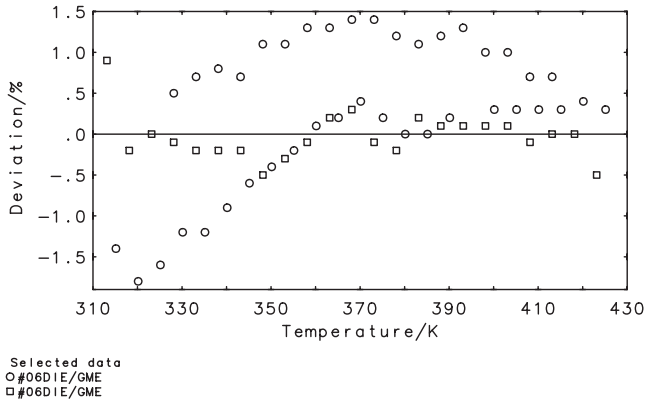

FIG. 173. Deviation plot for 1-butyl-4-dimethylaminopyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-037).

Parameters of regression polynomial (75.37.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	64	64	0.225	6.43−1	0.76	1.66−1	17

T/K	A_1	A_2	A_3	A_4	Uncert.
313.1–425.1	9.274 66+1	−1.028 57+1	2.190 75		IV

Deviation plot for 1-Butyl-4-dimethylaminopyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-037) is given in Fig. 173.

6.8.7.38. 1-Hexyl-2,3-dimethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (75-038)

Name:	1-Hexyl-2,3-dimethyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{13}H_{21}F_6N_3O_4S_2$
CAS-RN:	384347-22-2
Group No:	75-038

Experimental heat capacities (75.38.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	*p*	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.38.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	5.526 74+1	9.140 72			VI

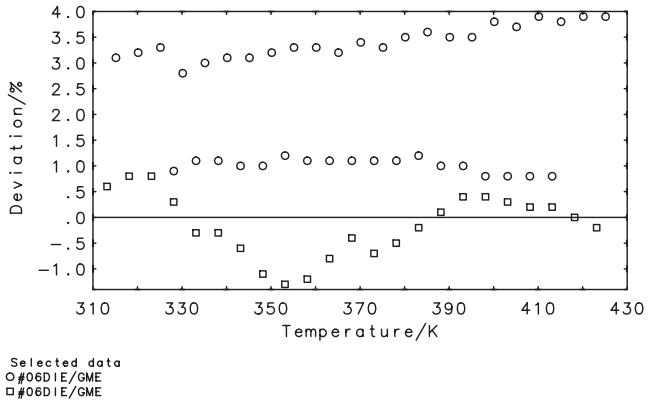

FIG. 174. Deviation plot for 1-octyl-3-methylimidazolium trifluoromethanesulfonate (75-039).

6.8.7.39. 1-Octyl-3-methylimidazolium trifluoromethanesulfonate (75-039)

Name: 1-Octyl-3-methylimidazolium trifluoromethanesulfonate

Formula: $C_{13}H_{23}F_3N_2O_3S$
CAS-RN: 403842-84-2
Group No: 75-039

Experimental heat capacities (75.39.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	p	BDHT	2004KIM/SHI
2006DIE/GME		313.2–423.1	23	n/a	n/a	n/a	p	BDCT	2000BEC/AUF

Correlated heat capacities (75.39.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.530	2.05	2.65	1.81	41
2006DIE/GME	313.2–423.1	23	1.00	#	0.617	4.48−1	0.62	−1.16−1	−3

Parameters of regression polynomial (75.39.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	64	64	0.572	1.69	2.19	1.12	38

T/K	A_1	A_2	A_3	A_4	Uncert.
313.2–425.1	4.696 98+1	7.437 21			IV

Deviation plot for 1-Octyl-3-methylimidazolium trifluoromethanesulfonate (75-039) is given in Fig. 174.

6.8.7.40. 1-Butyl-3-methyl-1*H*-imidazolium 2-(2-methoxyethoxy)ethyl sulfate (75-040)

Name: 1-Butyl-3-methyl-1*H*-imidazolium 2-(2-methoxyethoxy)ethyl sulfate

Formula: $C_{13}H_{26}N_2O_6S$
CAS-RN: 595565-54-1
Group No: 75-040

Experimental heat capacities (75.40.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.40.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	6.443 22+1	4.329 80			VI

6.8.7.41. 1-Hexyl-3-methylpyridinium 1,1,1-trifluoro-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-041)

Name:	1-Hexyl-3-methylpyridinium 1,1,1-trifluoro-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{14}H_{20}F_6N_2O_4S_2$
CAS-RN:	547718-92-3
Group No:	75-041

Experimental heat capacities (75.41.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.41.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	4.637 70+1	9.621 77			VI

6.8.7.42. 1-Methyl-3-octyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-042)

Name:	1-Methyl-3-octyl-1*H*-imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{14}H_{23}F_6N_3O_4S_2$
CAS-RN:	178631-04-4
Group No:	75-042

Experimental heat capacities (75.42.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.42.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	4.568 41+1	1.106 51+1			VI

6.8.7.43. 1-Hexyl-3,5-dimethylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-043)

Name:	1-Hexyl-3,5-dimethylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{15}H_{22}F_6N_2O_4S_2$
CAS-RN:	872672-54-3
Group No:	75-043

Experimental heat capacities (75.43.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.43.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	1.005 48+1	2.164 90+1			VI

6.8.7.44. 4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-044)

Name:	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{15}H_{23}F_6N_3O_4S_2$
CAS-RN:	872672-57-6
Group No:	75-044

Experimental heat capacities (75.44.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO
2006DIE/GME		315.1–425.1	41	5.00	n/a	n/a	p	BDHT	2004KIM/SHI
2006DIE/GME		313.1–418.1	22	n/a	n/a	n/a	p	BDCT	2000BEC/AUF

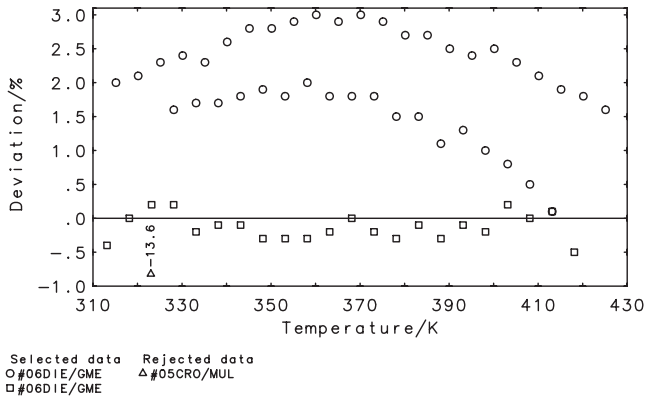

FIG. 175. Deviation plot for 4-(dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-044).

Correlated heat capacities (75.44.2)

Reference	T/K	nPts	$\sigma_r C$/%		d_w	d/R	d_r/%	d_b/R	+/−
2006DIE/GME	315.1–425.1	41	5.00		0.423	1.99	2.11	1.88	41
2006DIE/GME	313.1–418.1	22	1.00	#	0.241	2.21−1	0.24	−1.33−1	−12

Rejected data: Reference (d/R, d_r, d_b/R, +/−)

2005CRO/MUL	(1.06+1, 13.60, −1.06+1, −1)

Parameters of regression polynomial (75.44.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−
p	65	63	0.379	1.65	1.75	1.18	29

T/K	A_1	A_2	A_3	A_4	Uncert.
313.1–425.1	1.036 86+2	−1.467 35+1	3.117 06		IV

Deviation plot for 4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-044) is given in Fig. 175.

6.8.7.45. 3-(Butoxycarbonyl)-1-butylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanensulfonamide (75-045)

Name:	3-(Butoxycarbonyl)-1-butylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{16}H_{22}F_6N_2O_6S_2$
CAS-RN:	872672-53-2
Group No:	75-045

Experimental heat capacities (75.45.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.45.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	5.635 97+1	9.621 73			VI

6.8.7.46. 3-Methyl-1-octylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-046)

Name:	3-Methyl-1-octylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{16}H_{24}F_6N_2O_4S_2$
CAS-RN:	712355-02-7
Group No:	75-046

Experimental heat capacities (75.46.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.46.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	4.605 46+1	1.154 61+1			VI

6.8.7.47. 4-(Dimethylamino)-1-hexyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (75-047)

Name:	4-(Dimethylamino)-1-hexyl-3-methylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide
Formula:	$C_{16}H_{25}F_6N_3O_4S_2$
CAS-RN:	872672-59-8
Group No:	75-047

Experimental heat capacities (75.47.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.47.3)

Type	nTot	nPts	s_w	s/R	$s_r/\%$	s_b/R	+/−
p	2	2	0.000	0.00	0.00	0.00	0

T/K	A_1	A_2	A_3	A_4	Uncert.
298.0–323.0	3.128 52+1	1.876 24+1			VI

6.8.7.48. 3,5-Diethyl-1-hexyl-2-propylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (75-048)

Name: 3,5-Diethyl-1-hexyl-2-propylpyridinium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide

Formula: $C_{20}H_{32}F_6N_2O_4S_2$
CAS-RN: 872672-56-5
Group No: 75-048

Experimental heat capacities (75.48.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.48.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	2	2	0.000	0.00	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.0–323.0		4.481 82+1		1.587 59+1				VI

6.8.7.49. *N*-[2-[2-(2-Hydroxyethoxy)ethoxy]ethyl]-*N*-[(2-hydroxyethoxy)ethyl]-*N*-methyl-1-tridecanaminium methylsulfate (75-049)

Name: *N*-[2-[2-(2-Hydroxyethoxy)ethoxy]ethyl]-*N*-[(2-hydroxyethoxy)ethyl]-*N*-methyl-1-tridecanaminium methylsulfate

Formula: $C_{25}H_{55}NO_9S$
CAS-RN: 872672-63-4
Group No: 75-049

Experimental heat capacities (75.49.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0–323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.49.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	2	2	0.000	0.00	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.0–323.0		8.233 36+1		1.539 48+1				VI

6.8.7.50. *N*,*N*,*N*-Tributyl-1-butanaminium 1,4-bis(2-ethylhexyl)sulfobutanedioate (75-050)

Name: *N*,*N*,*N*-Tributyl-1-butanaminium 1,4-bis(2-ethylhexyl)sulfobutanedioate

Formula: $C_{36}H_{73}NO_7S$
CAS-RN: 663955-05-3
Group No: 75-050

Experimental heat capacities (75.50.1)

Reference	Note	T/K	nPts	Err/%	Pur/%	Method	Type	Calor.	Cal. Reference
2005CRO/MUL		298.0323.0	2	5.00	n/a	n/a	p	BDHT	2004FRE/CRO

Parameters of regression polynomial (75.50.3)

Type	nTot	nPts	s_w	s/R	s_r/%	s_b/R	+/−	
p	2	2	0.000	0.00	0.00	0.00	0	
T/K		A_1		A_2		A_3	A_4	Uncert.
298.0–323.0		7.334 19+1		2.886 54+1				VI

The following list presents only references referred to in this work. The references were taken from a complete database covering all compiled data presented both previously in Monograph No. 6 (1996ZAB/RUZ) and Supplement I (2001ZAB/RUZ) and presently in this work. Thus, some references in the series YYYYAAA/BBB1 to YYYYAAA/BBBM, where M is from 2 up to 9 depending upon the number of identical references published by the same author(s) within the same year, may be missing as they refer to papers not included in this work.

7. Acknowledgments

This work was supported by the Ministry of Education of the Czech Republic under Grant No. MSM 6046137307 and by the Grant Agency of the Academy of Sciences of the Czech Republic under Grant No. IAA 400720710 and was carried out as IUPAC Physical and Biophysical Chemistry Division Project No. 2004-010-3-100.

8. References

1877BER M. Berthelot, C. R. Hebd. Seances Acad. Sci. **85**, 648 (1877).
1879BER M. Berthelot, C. R. Hebd. Seances Acad. Sci. **89**, 119 (1879).
1881VON M. A. von Reis, Ann. Phys. **13**, 447 (1881).
1886LUD C. Ludeking, Ann. Phys. **27**, 72 (1886).
1886SCH R. Schiff, Justus Liebigs Ann. Chem. **233**, 300 (1886).
1887SCH R. Schiff, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **1**, 376 (1887).
1890PIC S. U. Pickering, Proc. R. Soc. London **49**, 11 (1890).
1894BRU L. Bruner, Ber. Dtsch. Chem. Ges. **27**, 2102 (1894).
1895PIC S. U. Pickering, J. Chem. Soc. **67**, 664 (1895).
1898LOU W. Louguinine, Ann. Chim. Phys. **13**, 289 (1898).
1900LOU W. Louguinine, Arch. Sci. Phys. Nat. **9**, 5 (1900).
1901DEF M. De Forcrand, C. R. Hebd. Seances Acad. Sci. **132**, 569 (1901).
1901KAH L. Kahlenberg, J. Phys. Chem. **5**, 284 (1901).
1902LOU1 W. Louguinine, Ann. Chim. Phys. **26**, 228 (1902).
1902LOU2 W. Louguinine, Ann. Chim. Phys. **27**, 105 (1902).
1907BAT A. Battelli, Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend. **16**, 243 (1907).
1907GUI2 M. Guinchant, C. R. Hebd. Seances Acad. Sci. **145**, 320 (1907).
1907WAL P. Walden, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **58**, 479 (1907).
1908BOG/WIN A. Bogojawlensky and N. Winogradow, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **64**, 251 (1908).
1909GOO/KAL H. M. Goodwin and H. T. Kalmus, Phys. Rev. **28**, 1 (1909).
1909SCH F. Schwers, Recl. Trav. Chim. Pays-Bas **28**, 42 (1909).
1911LEW/RAN G. N. Lewis and M. Randall, J. Am. Chem. Soc. **33**, 476 (1911).
1912BAU M. E. Baud, Ann. Chim. Phys. **27**, 89 (1912).
1912LUS S. Lussana, Nuovo Cimento **4**, 207 (1912).
1912SCH1 A. Schulze, Ber. Dtsch. Chem. Ges. **14**, 189 (1912).
1912SCH2 A. Schulze, Ber. Dtsch. Chem. Ges. **14**, 258 (1912).
1913CAM A. Campetti, Atti Accad. Sci. Torino, Cl. Sci. Fis., Mat. Nat. **48**, 968 (1913).
1913HER/RAT W. Herz and W. Rathmann, Chem. Ztg. **37**, 621 (1913).
1913NAS/BRE2 R. Nasini and U. Bresciani, Gazz. Chim. Ital. **43**, 281 (1913).
1916BRA A. Bramley, J. Chem. Soc. **1916**, 496 (1916).
1917HIL/DUS J. H. Hildebrand, A. D. Duschak, A. H. Foster, and C. W. Beebe, J. Am. Chem. Soc. **39**, 2293 (1917).
1918NAR J. Narbutt, Z. Elektrochem. **24**, 339 (1918).
1919DEJ M. G. Dejardin, Ann. Phys. (Paris) **11**, 253 (1919).
1920COH/MOE E. Cohen and A. L. T. Moesveld, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **95**, 305 (1920).
1920GIB/LAT G. E. Gibson, W. M. Latimer, and G. S. Parks, J. Am. Chem. Soc. **42**, 1533 (1920).
1920GIB/PAR G. E. Gibson, G. S. Parks, and W. M. Latimer, J. Am. Chem. Soc. **42**, 1542 (1920).
1921TRE R. Trehin, Ann. Phys. (Paris) **15**, 246 (1921).
1922HER/SCH W. Herz and P. Schuftan, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **101**, 269 (1922).
1924GAR/RAN W. E. Garner and F. C. Randall, J. Chem. Soc. **1924**, 881 (1924).
1924HER/BLO W. Herz and W. Bloch, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **110**, 23 (1924).
1924WIL/DAN J. W. Williams and F. Daniels, J. Am. Chem. Soc. **46**, 903 (1924).
1925DRU/WEI C. Drucker and H. Weissbach, Z. Phys. Chem., Stoechiom. Verwandtschaftsl. **117**, 209 (1925).
1925PAR G. S. Parks, J. Am. Chem. Soc. **47**, 338 (1925).
1925PAR/KEL G. S. Parks and K. K. Kelley, J. Am. Chem. Soc. **47**, 2089 (1925).
1925WIL J. W. Williams, J. Am. Chem. Soc. **47**, 2644 (1925).
1925WIL/DAN J. W. Williams and F. Daniels, J. Am. Chem. Soc. **47**, 1490 (1925).
1926AND/LYN D. H. Andrews, G. Lynn, and J. Johnston, J. Am. Chem. Soc. **48**, 1274 (1926).
1926PAR/AND G. S. Parks and C. T. Anderson, J. Am. Chem. Soc. **48**, 1506 (1926).
1926PAR/HUF G. S. Parks and H. M. Huffman, J. Am. Chem. Soc. **48**, 2788 (1926).
1927PAR/HUF G. S. Parks and H. M. Huffman, J. Phys. Chem. **31**, 1842 (1927).
1928LAN H. R. Lang, Proc. R. Soc. London, Ser. A **118**, 138 (1928).

1928LAT/GRE W. M. Latimer and B. S. Greensfelder, J. Am. Chem. Soc. **50**, 2202 (1928).
1928PAR/KEL G. S. Parks and K. K. Kelley, J. Phys. Chem. **32**, 734 (1928).
1929HER/LOR W. Herz and E. Lorentz, Z. Phys. Chem. Abt. A **140**, 406 (1929).
1929KEL1 K. K. Kelley, J. Am. Chem. Soc. **51**, 180 (1929).
1929KEL2 K. K. Kelley, J. Am. Chem. Soc. **51**, 779 (1929).
1929KEL3 K. K. Kelley, J. Am. Chem. Soc. **51**, 1145 (1929).
1929KEL5 K. K. Kelley, J. Am. Chem. Soc. **51**, 2738 (1929).
1929MIT/HAR1 S. Mitsukuri and K. Hara, Bull. Chem. Soc. Jpn. **4**, 77 (1929).
1930BAR/MAA W. H. Barnes and O. Maass, Can. J. Res. **3**, 70 (1930).
1930HUF/PAR1 H. M. Huffman, G. S. Parks, and A. C. Daniels, J. Am. Chem. Soc. **52**, 1547 (1930).
1930PAR/HUF1 G. S. Parks and H. M. Huffman, J. Am. Chem. Soc. **52**, 4381 (1930).
1930PAR/HUF2 G. S. Parks, H. M. Huffman, and S. B. Thomas, J. Am. Chem. Soc. **52**, 1032 (1930).
1930SOU/AND J. C. Southard and D. H. Andrews, J. Franklin Inst. **209**, 349 (1930).
1931BLA/LEI F. E. Blacet, P. A. Leighton, and E. P. Bartlett, J. Phys. Chem. **35**, 1935 (1931).
1931CLI/AND J. K. Cline and D. H. Andrews, J. Am. Chem. Soc. **53**, 3668 (1931).
1931DEE R. F. Deese, Jr., J. Am. Chem. Soc. **53**, 3673 (1931).
1931FIO/GIN E. F. Fiock, D. C. Ginnings, and W. B. Holton, Bur. Stand. J. Res. **6**, 881 (1931).
1931HUF/PAR H. M. Huffman, G. S. Parks, and M. Barmore, J. Am. Chem. Soc. **53**, 3876 (1931).
1931SMI/AND1 R. H. Smith and D. H. Andrews, J. Am. Chem. Soc. **53**, 3644 (1931).
1931THO/PAR S. B. Thomas and G. S. Parks, J. Phys. Chem. **35**, 2091 (1931).
1932NEU M. B. Neumann, Z. Phys. Chem. Abt. A **158**, 258 (1932).
1932NEU/KUR M. B. Neumann and I. A. Kurlyankin, Zh. Obshch. Khim. **2**, 317 (1932).
1932SPA/THO M. E. Spaght, S. B. Thomas, and G. S. Parks, J. Phys. Chem. **36**, 882 (1932).
1933FER/MIL A. Ferguson and J. T. Miller, Proc. Phys. Soc. London **45**, 194 (1933).
1933FER/THO J. D. Ferry and S. B. Thomas, J. Phys. Chem. **37**, 253 (1933).
1933KOL/UDO N. A. Kolosovskii and V. V. Udovenko, C. R. Hebd. Seances Acad. Sci. **197**, 519 (1933).
1933LEB/MOE M. LeBlanc and E. Moebius, Ber. Verh. Saechs. Akad. Wiss. Leipzig, Math.-Phys. Kl. **85**, 75 (1933).
1933PAR/HUF G. S. Parks, H. M. Huffman, and M. Barmore, J. Am. Chem. Soc. **55**, 2733 (1933).
1933ROT/MEY1 W. A. Roth and I. Meyer, Z. Elektrochem. **39**, 35 (1933).
1933ROT/MEY2 W. A. Roth, I. Meyer, and H. Zeumer, Z. Anorg. Allg. Chem. **214**, 309 (1933).
1933SOU/BRI J. C. Southard and F. G. Brickwedde, J. Am. Chem. Soc. **55**, 4378 (1933).
1933TRE/WAT V. C. G. Trew and G. M. C. Watkins, Trans. Faraday Soc. **29**, 1310 (1933).
1934JAC/PAR C. J. Jacobs and G. S. Parks, J. Am. Chem. Soc. **56**, 1513 (1934).
1934KOL/UDO2 N. A. Kolosovskii and V. V. Udovenko, Zh. Obshch. Khim. **4**, 1027 (1934).
1934LON/REY J. S. Long, J. B. Reynolds, and J. Napravnik, Ind. Eng. Chem. **26**, 864 (1934).
1934PAR/LIG G. S. Parks and D. W. Light, J. Am. Chem. Soc. **56**, 1511 (1934).
1934RAD/JUL D. Radulescu and O. Jula, Z. Phys. Chem. Abt. A **26**, 390 (1934).
1934ROT/MEY W. A. Roth, I. Meyer, and H. Zeumer, Z. Anorg. Allg. Chem. **216**, 303 (1934).
1935AOY/KAN S. Aoyama and E. Kanda, Sci. Rep. Tohoku Imp. Univ., Ser. 1 **24**, 116 (1935).
1935BAR/CLU E. Bartholome and K. Clusius, Z. Phys. Chem. Abt. B **28**, 167 (1935).
1935BRO/BAR1 R. S. Brown, W. H. Barnes, and O. Maass, Can. J. Res. **12**, 699 (1935).
1935BRO/BAR2 R. S. Brown, W. H. Barnes, and O. Maass, Can. J. Res. **13**, 167 (1935).
1935JAC L. Jacobs, Trans. Faraday Soc. **31**, 813 (1935).
1936ERN/WAT R. C. Ernst, C. H. Watkins, and H. H. Ruwe, J. Phys. Chem. **40**, 627 (1936).
1936EVA/EDL T. W. Evans and K. R. Edlund, Ind. Eng. Chem. **28**, 1186 (1936).
1936GIA/STO W. F. Giauque and J. W. Stout, J. Am. Chem. Soc. **58**, 1144 (1936).
1936KIN/GAR A. M. King and W. E. Garner, J. Chem. Soc. **127**, 1372 (1936).
1936KUR/VOS N. S. Kurnakov and N. K. Voskresenskaya, Izv. Akad. Nauk SSSR, Ser. Khim. 439 (1936).
1936LON/KEM E. A. Long and I. D. Kemp, J. Am. Chem. Soc. **58**, 1829 (1936).
1936PAR/TOD1 G. S. Parks, S. S. Todd, and W. A. Moore, J. Am. Chem. Soc. **58**, 398 (1936).
1937COH/BUI E. Cohen and J. S. Buij, Z. Phys. Chem. Abt. B **35**, 270 (1937).
1937ELL C. D. Ellyett, Trans. Faraday Soc. **33**, 1218 (1937).
1937GIA/EGA W. F. Giauque and C. J. Egan, J. Chem. Phys. **5**, 45 (1937).
1937STU D. R. Stull, J. Am. Chem. Soc. **59**, 2726 (1937).
1937VOL R. D. Vold, J. Am. Chem. Soc. **59**, 1515 (1937).
1938PAN/DUD N. Panov and I. Dudnikov, Sb. Tr. Opytnogo Zavoda im. Akad. S. V. Lebedeva **1938**, 36; from Chem. Abstr. **34**, 1514 (1940).
1939AST/EID1 J. G. Aston and M. L. Eidinoff, J. Am. Chem. Soc. **61**, 1533 (1939).
1939BYK V. T. Bykov, Zh. Fiz. Khim. **13**, 1013 (1939).
1939MAZ3 J. Mazur, Z. Phys. **113**, 710 (1939).
1939PHI N. M. Philip, Proc. Indian Acad. Sci., Sect. A **9**, 109 (1939).
1939RAI W. E. Railing, J. Am. Chem. Soc. **61**, 3349 (1939).
1939SAG/EVA B. H. Sage, H. D. Evans, and W. N. Lacey, Ind. Eng. Chem. **31**, 763 (1939).
1940COC/FER A. H. Cockett and A. Ferguson, Philos. Mag. **29**, 185 (1940).
1940MAZ J. Mazur, Acta Phys. Pol. **8**, 6 (1940).
1940MES/KEN G. H. Messerly and R. M. Kennedy, J. Am. Chem. Soc. **62**, 2988 (1940).
1940PIT1 K. S. Pitzer, J. Am. Chem. Soc. **62**, 331 (1940).
1940PIT2 K. S. Pitzer, J. Am. Chem. Soc. **62**, 1224 (1940).
1941SCH W. R. Schmidt, Ph.D. Thesis, Washington University (St. Louis), 1941.
1941ZHD A. K. Zhdanov, Zh. Obshch. Khim. **11**, 471 (1941).
1942ZIE/AND W. T. Ziegler and D. H. Andrews, J. Am. Chem. Soc. **64**, 2482 (1942).
1943AST/SZA J. G. Aston, G. J. Szasz, and H. L. Fink, J. Am. Chem. Soc. **65**, 1135 (1943).
1943BAC/PER H. J. Backer and W. G. Perdok, Recl. Trav. Chim. Pays-Bas **62**, 533 (1943).
1943PIT/SCO K. S. Pitzer and D. W. Scott, J. Am. Chem. Soc. **65**, 803 (1943).
1943RUE/HUF R. A. Ruehrwein and H. M. Huffman, J. Am. Chem. Soc. **65**, 1620 (1943).
1944BAI/TOD A. E. Bailey, S. S. Todd, W. S. Singleton, and G. D. Oliver, J. Am. Oil Chem. Soc. **21**, 293 (1944).
1944EIB J. Eibert, Ph.D Thesis, Washington University, St. Louis, Missouri, 1944.
1944GUT/SPI G. B. Guthrie, Jr., R. W. Spitzer, and H. M. Huffman, J. Am. Chem. Soc. **66**, 2120 (1944).
1945SCO/BRI R. B. Scott and F. G. Brickwedde, J. Res. Natl. Bur. Stand. **35**, 501 (1945).
1945SCO/MEY R. B. Scott, C. H. Meyers, R. D. Rands, Jr., F. G. Brickwedde, and N. Bekkedahl, J. Res. Natl. Bur. Stand. **35**, 39 (1945).
1945ZHD A. K. Zhdanov, Zh. Obshch. Khim. **15**, 895 (1945).
1946DOU/HUF1 D. R. Douslin and H. M. Huffman, J. Am. Chem. Soc. **68**, 173 (1946).

1946DOU/HUF2 D. R. Douslin and H. M. Huffman, J. Am. Chem. Soc. **68**, 1704 (1946).
1947CHA/SIN G. H. Charbonne and W. S. Singleton, J. Am. Oil Chem. Soc. **24**, 140 (1947).
1947COR/GIN R. J. Corruccini and D. C. Ginnings, J. Am. Chem. Soc. **69**, 2291 (1947).
1947HUF H. M. Huffman, Chem. Rev. (Washington, D.C.) **40**, 1 (1947).
1947JON/GIA W. M. Jones and W. F. Giauque, J. Am. Chem. Soc. **69**, 983 (1947).
1947KUR V. Ya. Kurbatov, Zh. Obshch. Khim. **17**, 1999 (1947).
1947OSB/GIN N. S. Osborne and D. C. Ginnings, J. Res. Natl. Bur. Stand. **39**, 453 (1947).
1947PUS/FED N. A. Pushin, A. V. Fedjushkin, and B. Krgovic, Glas. Hem. Drus. Beograd (Bull. Chem. Soc. Beograd) **11**, 12 (1947).
1947SKU S. M. Skuratov, Kolloidn. Zh. **9**, 133 (1947).
1948BER/MEL S. Berman, A. A. Melnychuk, and D. F. Othmer, Ind. Eng. Chem. **40**, 1312 (1948).
1948EUC A. Eucken, Z. Elektrochem. Angew. Phys. Chem. **52**, 255 (1948).
1948GIN/COR D. C. Ginnings and R. J. Corruccini, Ind. Eng. Chem. **40**, 1990 (1948).
1948KUR V. Ya. Kurbatov, Zh. Obshch. Khim. **18**, 372 (1948).
1948OLI/EAT G. D. Oliver, M. Eaton, and H. M. Huffman, J. Am. Chem. Soc. **70**, 1502 (1948).
1948TSC1 H. Tschamler, Monatsch. Chem. **79**, 162 (1948).
1948TSC2 H. Tschamler, Monatsch. Chem. **79**, 223 (1948).
1948TSC3 H. Tschamler, Monatsch. Chem. **79**, 233 (1948).
1948TSC5 H. Tschamler, Monatsch. Chem. **79**, 499 (1948).
1948TSC6 H. Tschamler, Monatsch. Chem. **79**, 508 (1948).
1949DHO/JUN M. D'Hont and J. C. Jungers, Bull. Soc. Chim. Belg. **58**, 196 (1949).
1949LEE J. W. Leech, Proc. Phys. Soc. London, Sect. B **62**, 390 (1949).
1949PAR/MOO G. S. Parks, G. E. Moore, M. L. Renquist, B. F. Naylor, L. A. McClaine, P. S. Fujii, and J. A. Hatton, J. Am. Chem. Soc. **71**, 3386 (1949).
1949STA/GUP L. A. K. Staveley and A. K. Gupta, Trans. Faraday Soc. **45**, 50 (1949).
1949TSC/RIC1 H. Tschamler and E. Richter, Monatsch. Chem. **80**, 510 (1949).
1949TSC/RIC2 H. Tschamler, E. Richter, and F. Wettig, Monatsch. Chem. **80**, 749 (1949).
1949TSC/RIC3 H. Tschamler, E. Richter, and F. Wettig, Monatsch. Chem. **80**, 856 (1949).
1949TSC/WET H. Tschamler, F. Wettig, and E. Richter, Monatsch. Chem. **80**, 572 (1949).
1949WEI *Physical Methods of Organic Chemistry*, edited by A. Weissberger (Interscience, New York, 1949), Vol. 1, p. 773.
1949WUY/JUN J. Wuyts and J. C. Jungers, Bull. Soc. Chim. Belg. **58**, 80 (1949).
1950AUE/SAG C. E. Auerbach, B. H. Sage, and W. N. Lacey, Ind. Eng. Chem. **42**, 110 (1950).
1950CRO/SMY1 R. W. Crowe and C. P. Smyth, J. Am. Chem. Soc. **72**, 1098 (1950).
1950CRO/SMY2 R. W. Crowe and C. P. Smyth, J. Am. Chem. Soc. **72**, 4009 (1950).
1950GIN/DOU D. C. Ginnings, T. B. Douglas, and A. F. Ball, J. Res. Natl. Bur. Stand. **45**, 23 (1950).
1950HOU/MAS2 E. W. Hough, D. M. Mason, and B. H. Sage, J. Am. Chem. Soc. **72**, 5775 (1950).
1950KUR V. Ya. Kurbatov, Zh. Obshch. Khim. **20**, 1139 (1950).
1950KUS/CRO L. M. Kushner, R. W. Crowe, and C. P. Smyth, J. Am. Chem. Soc. **72**, 1091 (1950).
1950SAG/HOU B. H. Sage and E. W. Hough, Anal. Chem. **22**, 1304 (1950).
1951CON/SAG T. J. Connolly, B. H. Sage, and W. N. Lacey, Ind. Eng. Chem. **43**, 946 (1951).
1951EUC/EIG A. Eucken and M. Eigen, Z. Elektrochem. **55**, 343 (1951).
1951POP/GAL M. M. Popov and G. L. Gal'chenko, Zh. Obshch. Khim. **21**, 2220 (1951).
1951SIE/CRU L. Sieg, J. L. Crutzen, and W. Jost, Z. Phys. Chem. (Leipzig) **198**, 263 (1951).
1952ADA/JOH G. B. Adams, Jr., H. L. Johnston, and E. C. Kerr, J. Am. Chem. Soc. **74**, 4784 (1952).
1952CUR/JOH *Glycols*, edited by G. O. Curme, Jr., and F. Johnston (Reinhold, New York, 1952), p. 251.
1952SCH/SAG W. G. Schlinger and B. H. Sage, Ind. Eng. Chem. **44**, 2454 (1952).
1952STA/AMI R. D. Stallard and E. S. Amis, J. Am. Chem. Soc. **74**, 1781 (1952).
1953WES/HAT E. F. Westrum, Jr., J. B. Hatcher, and D. W. Osborne, J. Chem. Phys. **21**, 419 (1953).
1954FIN/GRO2 H. L. Finke, M. E. Gross, G. Waddington, and H. M. Huffman, J. Am. Chem. Soc. **76**, 333 (1954).
1954STR/ICK P. G. Strelkov, E. S. Ickevich, V. N. Kostryukov, G. G. Mirskaya, and V. N. Samoilov, Zh. Fiz. Khim. **28**, 459 (1954).
1955HUT/MAN E. Hutchinson and K. E. Manchester, Rev. Sci. Instrum. **26**, 364 (1955).
1955LYD A. L. Lydersen, University of Wisconsin, College of Engineering, Engineering Experimental Station Report 3, Madison, Wisconsin, 1955.
1955RUI1 L. H. Ruiter, Recl. Trav. Chim. Pays-Bas **74**, 1131 (1955).
1955RUI2 L. H. Ruiter, Recl. Trav. Chim. Pays-Bas **74**, 1467 (1955).
1955STA/TUP L. A. K. Staveley, W. I. Tupman, and K. R. Hart, Trans. Faraday Soc. **51**, 323 (1955).
1956DUF/EVE G. M. Duff and D. H. Everett, Trans. Faraday Soc. **52**, 753 (1956).
1956FIN/SCO H. L. Finke, D. W. Scott, M. E. Gross, J. F. Messerly, and G. Waddington, J. Am. Chem. Soc. **78**, 5469 (1956).
1956PAR/KEN G. S. Parks, W. D. Kennedy, R. R. Gates, J. R. Mosley, G. E. Moore, and M. L. Renquist, J. Am. Chem. Soc. **78**, 56 (1956).
1956POP/KOL M. M. Popov and V. P. Kolesov, Zh. Obshch. Khim. **26**, 2385 (1956).
1956SCH/GOT V. E. Schrock, R. E. Gott, and E. S. Starkman, Wright Air Development Center, Wright-Patterson Air Force Base, WADC Technical Report No. TR 56-104, Ohio, 1956.
1957CRU/JOS J. L. Crutzen, W. Jost, and L. Sieg, Ber. Bunsenges. Phys. Chem. **61**, 230 (1957).
1957KEN J. Kenttamaa, Suom. Kemistil. B **B30**, 15 (1957).
1957MCC/FIN2 J. P. McCullough, H. L. Finke, J. F. Messerly, S. S. Todd, T. C. Kincheloe, and G. Waddington, J. Phys. Chem. **61**, 1105–16 (1957).
1957PIL G. Pilcher, Anal. Chim. Acta **17**, 144 (1957).
1958GOO/SOL J. Goodkin, C. Solomons, and G. J. Janz, Rev. Sci. Instrum. **29**, 105 (1958).
1958HIL/KRA D. L. Hildenbrand, W. R. Kramer, R. A. McDonald, and D. R. Stull, J. Am. Chem. Soc. **80**, 4129 (1958).
1958MUR/VAN P. S. Murti and M. Van Winkle, Chem. Eng. Data Ser. **3**, 65 (1958).
1958PEP W. J. Peppel, Ind. Eng. Chem. **50**, 767 (1958).
1958SWI/ZIE1 W. Swietoslawski and A. Zielenkiewicz, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **6**, 365 (1958).
1958SWI/ZIE2 W. Swietoslawski and A. Zielenkiewicz, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **6**, 367 (1958).
1958WES/GIN E. D. West and D. C. Ginnings, J. Res. Natl. Bur. Stand. **60**, 309 (1958).
1959ABA/MUS A. K. Abas-Zade and R. A. Mustafaev, Dokl. Akad. Nauk Az. SSR **15**, 775 (1959).
1959BAK B. L. Baker, U.S. Atomic Energy Commission Report No. 38-1-118, U. S. Government Printing Office, Washington, D. C., 1959.
1959DEA/EVA G. H. Deal, Jr., H. D. Evans, E. D. Oliver, and M. N. Papadopoulos, Pet. Refin. **38**(9), 185 (1959).
1959HUT/BAI E. Hutchinson and L. G. Bailey, Z. Phys. Chem. (Munich) **21**, 30 (1959).
1959KEN/TOM J. Kenttamaa, E. Tommila, and M. Martti, Ann. Acad. Sci. Fenn., Ser. A2 No. 93, 1 (1959).
1959ONK U. Onken, Z. Elektrochem. **63**, 321 (1959).
1959RIB/EGO S. L. Ribkin and B. N. Egorov, At. Energ. **7**, 462 (1959).

1960KEN/LIN J. Kenttamaa and J. J. Lindberg, Suom. Kemistil. B **B33**, 32 (1960).
1960SWI/ZIE W. Swietoslawski and A. Zielenkiewicz, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **8**, 651 (1960).
1961GEL B. E. Geller, Zh. Fiz. Khim. **35**, 2210 (1961).
1961GOO R. D. Goodwin, J. Res. Natl. Bur. Stand., Sect. C **65C**, 231 (1961).
1961ROU R. A. Rousseau, Ph.D. thesis, John Hopkins University, 1961.
1962GOL/BEL M. H. Gollis, L. I. Belenyessy, B. J. Gudzinowicz, S. D. Koch, J. O. Smith, and R. J. Wineman, J. Chem. Eng. Data **7**, 311 (1962).
1962HAT/HIL W. E. Hatton, D. L. Hildenbrand, G. C. Sinke, and D. R. Stull, J. Chem. Eng. Data **7**, 229 (1962).
1962KAT T. Katayama, Kagaku Kogaku Ronbunshu **26**, 361 (1962).
1962KOL/PAU V. P. Kolesov, I. E. Paukov, and S. M. Skuratov, Zh. Fiz. Khim. **36**, 770 (1962).
1962MUR/YAM Y. Murakami and T. Yamada, Kagaku Kogaku Ronbunshu **26**, 867 (1962).
1962RAB/NIK I. B. Rabinovich and P. N. Nikolaev, Dokl. Akad. Nauk SSSR **142**, 1335 (1962).
1962SCO/GUT D. W. Scott, G. B. Guthrie, J. F. Messerly, S. S. Todd, W. T. Berg, I. A. Hossenlopp, and J. P. McCullough, J. Phys. Chem. **66**, 911 (1962).
1962SHE/NIN T. Sherlak and B. Ninkov, Glas. Hem. Tehnol. Bosne Hercegovine (Bull. Chem. Technol. Bosnia Herzegovina) **11**, 43 (1962); from Chem. Abstr. **61**, 2496d (1964).
1962VAL/BRO R. H. Valentine, G. E. Brodale, and W. F. Giauque, J. Phys. Chem. **66**, 392 (1962).
1963AND/COU1 R. J. L. Andon, J. F. Counsell, E. F. G. Herington, and J. F. Martin, Trans. Faraday Soc. **59**, 830 (1963).
1963AND/COU2 R. J. L. Andon, J. F. Counsell, and J. F. Martin, Trans. Faraday Soc. **59**, 1555 (1963).
1963BEN L. Benjamin, Can. J. Chem. **41**, 2210 (1963).
1963GUD/CAM B. J. Gudzinowicz, R. H. Campbell, and J. S. Adamas, J. Chem. Eng. Data **8**, 201 (1963).
1963JAN/KEL G. J. Janz and F. J. Kelly, J. Phys. Chem. **67**, 2848 (1963).
1963OET F. L. Oetting, J. Phys. Chem. **67**, 2757 (1963).
1964ARN1 H. Arnold, Z. Phys. Chem. (Leipzig) **225**, 45 (1964).
1964CAM/NAG A. N. Campbell and M. K. Nagarajan, Can. J. Chem. **42**, 1616 (1964).
1964MOE/THO E. A. Moelwyn-Hughes and P. L. Thorpe, Proc. R. Soc. London, Ser. A **278**, 574 (1964).
1964RAS/BAS R. P. Rastogi and P. S. Bassi, J. Phys. Chem. **68**, 2398 (1964).
1964SIN/OET G. C. Sinke and F. L. Oetting, J. Phys. Chem. **68**, 1354 (1964).
1965CAM/GIE A. N. Campbell and J. M. T. M. Gieskes, Can. J. Chem. **43**, 1004 (1965).
1965COU/GRE J. F. Counsell, J. H. S. Green, J. L. Hales, and J. F. Martin, Trans. Faraday Soc. **61**, 212 (1965).
1965COU/HAL J. F. Counsell, J. L. Hales, and J. F. Martin, Trans. Faraday Soc. **61**, 1869 (1965).
1995FIN/GRU G. H. Findenegg, K. Gruber, J. F. Pereira, and F. Kohler, Monatsch. Chem. **96**, 669 (1965).
1965KAU/BIT E. Kauer and H. J. Bittrich, Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer," Leuna-Merseburg **7**, 73 (1965).
1965MES/TOD2 J. F. Messerly, S. S. Todd, and H. L. Finke, J. Phys. Chem. **69**, 4304 (1965).
1965OET F. L. Oetting, J. Chem. Eng. Data **10**, 122 (1965).
1965STE/BLA K. F. Sterrett, D. H. Blackburn, A. B. Bestul, S. S. Chang, and J. Horman, J. Res. Natl. Bur. Stand., Sect. C **69C**, 19 (1965).
1965STE/CAL F. Steckel, E. Calvet, and A. Cagnasso, C. R. Hebd. Seances Acad. Sci. **261**, 2095 (1965).
1965SUG/SEK H. Suga and S. Seki, Bull. Chem. Soc. Jpn. **38**, 1000 (1965).
1965TUN/MIS V. P. Tungusov and K. P. Mishchenko, Zh. Fiz. Khim. **39**, 2968 (1965).
1965ZIE A. Zielenkiewicz, Przem. Chem. **44**, 664 (1965).
1966BEA/CLE R. H. Beaumont, B. Clegg, G. Gee, J. B. M. Herbert, D. J. Marks, R. C. Roberts, and D. Sims, Polymer **7**, 401 (1966).
1966DRA/LAN S. I. Drakin, L. V. Lantukhova, and M. Kh. Karapet'yanc, Zh. Fiz. Khim. **40**, 451 (1966).
1966HWA/ZIE S. C. P. Hwa and W. T. Ziegler, J. Phys. Chem. **70**, 2572 (1966).
1966KLE I. Klesper, Z. Phys. Chem. **51**, 1 (1966).
1966NIK/LEB P. N. Nikolaev and B. V. Lebedev, Tr. Khim. Khim. Tekhnol. (2), 332 (1966).
1966NIK/RAB P. N. Nikolaev, I. B. Rabinovich, V. A. Galperin, and V. G. Cvetkov, Zh. Fiz. Khim. **40**, 1091 (1966).
1966PER/COM Perkin-Elmer DSC-1, commercial calorimeter, Anal. Chem. **38**, 1331 (1966).
1966SAV M. S. Savogina, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **9**, 379 (1966).
1967CHA/HOR S. S. Chang, J. A. Horman, and A. B. Bestul, J. Res. Natl. Bur. Stand., Sect. A **71A**, 293 (1967).
1967GRA R. W. Grabner, Ph.D. Thesis, Lehigh University, 1967.
1967MES/GUT J. F. Messerly, G. B. Guthrie, S. S. Todd, and H. L. Finke, J. Chem. Eng. Data **12**, 338 (1967).
1967NIK/RAB1 P. N. Nikolaev and I. B. Rabinovich, Zh. Obshch. Khim. **41**, 2191 (1967).
1967NIK/RAB2 P. N. Nikolaev, I. B. Rabinovich, and B. V. Lebedev, Zh. Fiz. Khim. **41**, 1294 (1967).
1967PAC P. Pacor, Anal. Chim. Acta **37**, 200 (1967).
1967RAS/GAN Yu. L. Rastorguev and Yu. A. Ganiev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **10**, 79 (1967).
1967SMI/GOO2 N. K. Smith and W. D. Good, J. Chem. Eng. Data **12**, 572 (1967).
1968AND/COU2 R. J. L. Andon, J. F. Counsell, and J. F. Martin, J. Chem. Soc. A **1968**, 1894.
1968CLE/MEL G. A. Clegg, T. P. Melia, and A. Tyson, Polymer **9**, 75 (1968).
1968COU/LEE J. F. Counsell, E. B. Lees, and J. F. Martin, J. Chem. Soc. A **1968**, 1819.
1968OST/DOB V. E. Ostrovskii, N. N. Dobrovol'skii, I. R. Karpovich, and F. Ya. Frolov, Zh. Fiz. Khim. **42**, 550 (1968).
1968PAZ/REC M. I. Paz Andrade, E. Recacho, and J. M. Paz Fernandez, Acta Cient. Compostelana **5**, 49 (1968).
1968REC1 W. M. Recko, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **16**, 543 (1968).
1968WAD I. Wadso, Acta Chem. Scand. (1947-1973) **22**, 927 (1968).
1968WES/FUR E. F. Westrum, Jr., G. T. Furukawa, and J. P. McCullough, in *Experimental Thermodynamics*, edited by J. P. McCullough and D. W. Scott (Butterworth, London, 1968), Vol. 1, 133.
1968WES/WES E. D. West and E. F. Westrum, Jr., in *Experimental Thermodynamics*, edited by J. P. McCullough and D. W. Scott (Butterworth, London, 1968), Vol. 1, 333.
1969ATK/LAR C. M. L. Atkinson, J. A. Larkin, and M. J. Richardson, J. Chem. Thermodyn. **1**, 435 (1969).
1969BER/WES H. A. Berman and E. D. West, J. Chem. Eng. Data **14**, 107 (1969).
1969BOI/BRO E. Boitard, J.-P. Bros, and M. Lafitte, J. Chim. Phys. Phys.-Chim. Biol. **66**, 166 (1969).
1969CLE/MEL4 G. A. Clegg and T. P. Melia, Polymer **10**, 912 (1969).
1969PER/COM Perkin-Elmer DSC-2, commercial calorimeter, Prospectus, 1969.
1969WIL/ROT E. Wilhelm, E. Rott, and F. Kohler, *Proceedings of the First International Conference Calorimetry and Thermodynamics*, Warszaw, Poland, 1969, p. 767.
1969WIL/SCH E. Wilhelm, R. Schano, G. Becker, G. H. Findenegg, and F. Kohler, Trans. Faraday Soc. **65**, 1443 (1969).
1969YAG M. Sh. Yagfarov, Zh. Fiz. Khim. **43**, 1620 (1969).
1970AKH A. G. Akhmedov, Zh. Fiz. Khim. **44**, 2061 (1970).
1970ANO Anon, *Product Information of Dimethylformamide*, Du Pont de Nemours, Wilmington, DE, 1970; from G. Hradetzky, I. Hammerl, W. Kisan, K. Wehner, and H.-J. Bittrich, *Data of Selective Solvents* (VEB, Berlin, 1989).
1970CLE/WES H. L. Clever and E. F. Westrum, Jr., J. Phys. Chem. **74**, 1309 (1970).
1970GOU/GIR P. Goursot, H. L. Girdhar, and E. F. Westrum, Jr., J. Phys.

Chem. **74**, 2538 (1970).
1970HAR/HEA D. Harrop, A. J. Head, and G. B. Lewis, J. Chem. Thermodyn. **2**, 203 (1970).
1970KRE G. C. Kresheck, J. Chem. Phys. **52**, 5966 (1970).
1970LKB/COM LKB 8721-1, commercial calorimeter, Prospectus, 1970.
1970MAR/RAB L. Yu. Martynenko, I. B. Rabinovich, Yu. B. Ovchinnikov, and V. A. Maslova, Vysokomol. Soedin., Ser. A **12**, 841 (1970).
1970MES/FIN J. F. Messerly and H. L. Finke, J. Chem. Thermodyn. **2**, 867 (1970).
1970PAZ/PAZ M. I. Paz Andrade, J. M. Paz, and E. Recacho, An. Quim. **66**, 961 (1970).
1970REC W. M. Recko, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **18**, 297 (1970).
1971AMI/ALI Kh. I. Amirkhanov, B. G. Alibekov, D. I. Vikhrov, V. A. Mirskaya, and L. N. Levina, Teplofiz. Vys. Temp. **9**, 1310 (1971).
1971BOY/SAN R. H. Boyd, S. N. Sanwal, S. Shary-Tehrany, and D. McNally, J. Phys. Chem. **75**, 1264 (1971).
1971CAR/WES H. G. Carlson and E. F. Westrum, Jr., J. Chem. Phys. **54**, 1464 (1971).
1971DES/BHA D. D. Deshpande and L. G. Bhatgadde, Aust. J. Chem. **24**, 1817 (1971).
1971DU/COM Du Pont 990 DSC, commercial calorimeter, Prospectus, 1971.
1971GOP/GAM E. S. R. Gopal, R. D. Gambhir, K. Govindarajan, and B. Viswanathan, J. Indian Inst. Sci. **53**, 355 (1971).
1971HAL/BAL H. K. Hall, Jr. and J. H. Baldt, J. Am. Chem. Soc. **93**, 140 (1971).
1971KHA/SUB V. H. Khan and S. V. Subrahmanyam, Trans. Faraday Soc. **67**, 2282 (1971).
1971KON/SUU J. Konicek, J. Suurkuusk, and I. Wadso, Chem. Scr. **1**, 217 (1971).
1971KON/WAD J. Konicek and I. Wadso, Acta Chem. Scand. (1947-1973) **25**, 1541 (1971).
1971MAR/CIO D. I. Marchidan and M. Ciopec, Rev. Roum. Chim. **16**, 1145 (1971).
1971MUS R. A. Mustafaev, Izv. Vyssh. Ucheb. Zaved., Priborostr. **14**, 129 (1971).
1971PIC/LED P. Picker, P. A. Leduc, P. R. Philip, and J. E. Desnoyers, J. Chem. Thermodyn. **3**, 631 (1971).
1971REC/SAD W. M. Recko, K. W. Sadowska, and M. K. Woycicka, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **19**, 475 (1971).
1971VAN J. C. Van Miltenburg, Ph.D. thesis, Rijksuniversiteit Utrecht, 1971.
1971VAS/PET I. A. Vasil'ev, V. M. Petrov, V. M. Ignat'ev, and A. A. Vvedenskii, Zh. Fiz. Khim. **45**, 1316 (1971), data deposited in VINITI 2530–71.
1971WON/WES W.-K. Wong and E. F. Westrum, Jr., J. Chem. Thermodyn. **3**, 105 (1971).
1972COP/REA A. F. G. Cope, H. H. Reamer, and C. J. Pings, Ber. Bunsenges. Phys. Chem. **76**, 318 (1972).
1972FIN/MES H. L. Finke, J. F. Messerly, and S. S. Todd, J. Chem. Thermodyn. **4**, 359 (1972).
1972KAW/OTA F. Kawaizumi, T. Otake, H. Nomura, and Y. Miyahara, Nippon Kagaku Kaishi (10), 1773 (1972).
1972REC/SAD W. M. Recko and K. W. Sadowska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **20**, 73 (1972).
1972VAN J. C. Van Miltenburg, J. Chem. Thermodyn. **4**, 773 (1972).
1973AKH/EKS T. S. Akhundov and R. A. Eksaev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **16**, 68 (1973).
1973HAL/SMI H. K. Hall, Jr., C. D. Smith, and J. H. Baldt, J. Am. Chem. Soc. **95**, 3197 (1973).
1973KAL/WOY B. Kalinowska and M. Woycicka, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **21**, 845 (1973).
1973KIS/SUG K. Kishimoto, H. Suga, and S. Seki, Bull. Chem. Soc. Jpn. **46**, 3020 (1973).
1973KUS/SUU K. Kusano, J. Suurkuusk, and I. Wadso, J. Chem. Thermodyn. **5**, 757 (1973).
1973MOS/NIK E. M. Moseeva, P. N. Nikolaev, T. A. Sechenova, and I. B. Rabinovich, Tr. Khim. Khim. Tekhnol. **32**, 153 (1973).
1973PER/COM Perkin-Elmer DSC-1-B, commercial calorimeter, Prospectus, 1973.
1973SUB/RAJ S. V. Subrahmanyam and E. Rajagopal, Z. Phys. Chem. (Munich) **85**, 256 (1973).
1973VAS/KOR I. A. Vasil'ev and A. D. Korkhov, Zh. Fiz. Khim. **47**, 2710 (1973), data deposited in VINITI 6326-73.
1974AND/COU R. J. L. Andon, J. F. Counsell, D. A. Lee, and J. F. Martin, J. Chem. Soc., Faraday Trans. 1 **70**, 1914 (1974).
1974ATA/CHI T. Atake and H. Chihara, Bull. Chem. Soc. Jpn. **47**, 2126 (1974).
1974DEV/SOM C. De Visser and G. Somsen, Z. Phys. Chem. (Munich) **92**, 159 (1974).
1974DIA/REN M. Diaz Pena and J. A. R. Renuncio, An. Quim. **70**, 113 (1974).
1974MOS/MOU C. Mosselman, J. Mourik, and H. Dekker, J. Chem. Thermodyn. **6**, 477 (1974).
1974PET/TER J. C. Petit and L. Ter Minassian, J. Chem. Thermodyn. **6**, 1139 (1974).
1974RAJ/SUB E. Rajagopal and S. V. Subrahmanyam, J. Chem. Thermodyn. **6**, 873 (1974).
1974SUU/WAD J. Suurkuusk and I. Wadso, J. Chem. Thermodyn. **6**, 667 (1974).
1974WIL/ZET E. Wilhelm, M. Zettler, and H. Sackmann, Ber. Bunsenges. Phys. Chem. **78**, 795 (1974).
1975AND/MAR R. J. L. Andon and J. F. Martin, J. Chem. Thermodyn. **7**, 593 (1975).
1975BER/OLO S. Bergstrom and G. Olofsson, J. Solution Chem. **4**, 535 (1975).
1975GRI/RAS B. A. Grigor'ev, Yu. L. Rastorguev, and G. S. Yanin, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **18**, 63 (1975).
1975GRO/BEN J.-P. E. Grolier, G. C. Benson, and P. Picker, J. Chem. Eng. Data **20**, 243 (1975).
1975HOL/ZIE J. K. Holzhauer and W. T. Ziegler, J. Phys. Chem. **79**, 590 (1975).
1975JOL/BOI C. Jolicoeur, J. Boileau, S. Bazinet, and P. Picker, Can. J. Chem. **53**, 716 (1975).
1975MEK/KAR S. A. Mekhtiev, K. A. Karasharli, and O. I. Dzhafarov, Zh. Fiz. Khim. **49**, 259 (1975), data deposited in VINITI 2585-74.
1975NIC/WAD N. Nichols and I. Wadso, J. Chem. Thermodyn. **7**, 329 (1975).
1975PED/KAY M. J. Pedersen, W. B. Kay, and H. C. Hershey, J. Chem. Thermodyn. **7**, 1107 (1975).
1975RAS/GRI Yu. L. Rastorguev, B. A. Grigor'ev, and G. S. Yanin, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **18**, 73 (1975).
1975SAF/GER L. I. Safir, A. A. Gerasimov, and B. A. Grigor'ev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **18**, 61 (1975).
1975SAN J. L. San Jose, Ph.D. thesis, Massachussetts Institute of Technology, 1975.
1975VYU/ZVE A. I. V'yugin, V. A. Zverev, and A. G. Krestov, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **18**, 1974 (1975).
1975WOY/KAL M. K. Woycicka and B. Kalinowska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **23**, 759 (1975).
1976BON/CER O. D. Bonner and P. J. Cerutti, J. Chem. Thermodyn. **8**, 105 (1976).
1976CON/GIA G. Conti, P. Gianni, E. Matteoli, and M. Mengheri, Chem. Ind. **58**, 225 (1976).
1976FOR/BEN1 J.-L. Fortier and G. C. Benson, J. Chem. Thermodyn. **8**, 411 (1976).
1976FOR/BEN2 J.-L. Fortier, G. C. Benson, and P. Picker, J. Chem. Thermodyn. **8**, 289 (1976).
1976GOO/LEE W. D. Good and S. H. Lee, J. Chem. Thermodyn. **8**, 643 (1976).
1976KAR/GRO M. H. Karbalai Ghassemi and J.-P. E. Grolier, Int. Data Ser., Sel. Data Mixtures, Ser. A (2), 95 (1976).
1976LEB/LIT B. V. Lebedev and V. Ya. Lityagov, Tr. Khim. Khim. Tekhnol. **5**, 89 (1976).
1976MAS/PET A. K. M. Masood and R. A. Pethrick, J. Chem. Soc., Faraday Trans. 1 **72**, 20 (1976).
1976MUS R. A. Mustafaev, Zh. Fiz. Khim. **50**, 1899 (1976), data deposited in VINITI 1224-76.
1976NIC/SKO N. Nichols, R. Skold, C. Spink, and I. Wadso, J. Chem. Thermodyn. **8**, 993 (1976).

1976PHI/MAT J. C. Phillips and M. M. Mattamal, J. Chem. Eng. Data **21**, 228 (1976).
1976SAN/MEL J. L. San Jose, G. Mellinger, and R. C. Reid, J. Chem. Eng. Data **21**, 414 (1976).
1976SKO/SUU R. Skold, J. Suurkuusk, and I. Wadso, J. Chem. Thermodyn. **8**, 1075 (1976).
1976VAS/KOR I. A. Vasil'ev, A. D. Korkhov, G. M. Minkin, I. B. Rabinovich, M. S. Sheiman, and V. P. Nistratov, Termodin. Org. Soedin. (5), 21 (1976).
1977BEL/BUB V. P. Belousov, V. Bubnov, R. Pfestorf, and A. Schumichen, Z. Chem. **17**, 382 (1977).
1977BON/BED O. D. Bonner, J. M. Bednarek, and R. K. Arisman, J. Am. Chem. Soc. **99**, 2898 (1977).
1977DEV/PER1 C. De Visser, G. Perron, and J. E. Desnoyers, Can. J. Chem. **55**, 856 (1977).
1977DEV/PER2 C. De Visser, G. Perron, and J. E. Desnoyers, J. Am. Chem. Soc. **99**, 5894 (1977).
1977DEV/PER3 C. De Visser, G. Perron, J. E. Desnoyers, W. J. M. Heuvelsland, and G. Somsen, J. Chem. Eng. Data **22**, 74 (1977).
1977FIN/MES H. L. Finke, J. F. Messerly, S. H. Lee, A. G. Osborn, and D. R. Douslin, J. Chem. Thermodyn. **9**, 937 (1977).
1977FOR/BEN J.-L. Fortier and G. C. Benson, J. Chem. Thermodyn. **9**, 1181 (1977).
1977HAI/SUG2 O. Haida, H. Suga, and S. Seki, J. Chem. Thermodyn. **9**, 1133 (1977).
1977HOF/SAN S. P. Hoffman, J. L. San Jose, and R. C. Reid, J. Chem. Eng. Data **22**, 385 (1977).
1977KU/COM KU-300, commercial calorimeter VNIIFTRI (soviet production), Termodin. Org. Soedin. (6), 89 (1977).
1977KUL/DZH2 A. M. Kuliev, O. I. Dzhafarov, K. A. Karasharli, and A. G. Kuznetsova, Zh. Fiz. Khim. **51**, 1564 (1977), data deposited in VINITI 987-77.
1977MUR/SUB N. M. Murthy and S. V. Subrahmanyam, Indian J. Pure Appl. Phys. **15**, 485 (1977).
1977NAZ/MUS Ya. M. Naziev, M. R. Mustafaev, and A. A. Abasov, Proceedings of the Seventh Symposium on Thermophysics Properties, 1977 (unpublished), p. 525.
1977STE/WAT W. V. Steele and I. Watt, J. Chem. Thermodyn. **9**, 843 (1977).
1977VOR/PRI A. F. Vorob'ev, N. M. Privalova, and M. V. Rekharskii, Zh. Fiz. Khim. **51**, 1843 (1977).
1977VYU A. I. V'yugin, Ph.D Thesis, Ivanovo Chemical Technology Institute (IKhTI), Ivanovo, Russia, 1977. From V. P. Korolev, V. A. Kukharenko, and G. A. Krestov, Zh. Fiz. Khim. **60**, 1854 (1986).
1977WIL/GRO E. Wilhelm, J.-P. E. Grolier, M. H. Karbalai Ghassemi, and M. H. Ghassemi, Ber. Bunsenges. Phys. Chem. **81**, 925 (1977).
1978BYV/JAS Yu. A. Byval'tsev, B. V. Jasiunas, and V. M. Perelygin, Izv. Vyssh. Uchebn. Zaved., Pishch. Tekhnol. (5), 169 (1978).
1978DEV/HEU C. De Visser, W. J. M. Heuvelsland, L. A. Dunn, and G. Somsen, J. Chem. Soc., Faraday Trans. 1 **74**, 1159 (1978).
1978GOO/SCO W. D. Good, D. W. Scott, S. Lee-Bechtold, and A. G. Osborn, U.S. Department of Energy Report, NIPER Report No. 1, National Institute for Petroleum and Energy Research, Bartlesville, Oklahoma, 1978.
1978GRO/WIL J.-P. E. Grolier, E. Wilhelm, and M. H. Hamedi, Ber. Bunsenges. Phys. Chem. **82**, 1282 (1978).
1978LEB/RAB2 B. V. Lebedev, I. B. Rabinovich, V. I. Milov, and V. Ya. Lityagov, J. Chem. Thermodyn. **10**, 321 (1978).
1978MAR/CIO1 D. I. Marchidan and M. Ciopec, J. Therm. Anal. **14**, 131 (1978).
1978MIL K. C. Mills, Thermochim. Acta **23**, 390 (1978).
1978MOY/SAS C. T. Moynihan, H. Sasabe, D. S. Czaplak, and U. E. Schnaus, J. Chem. Eng. Data **23**, 107 (1978).
1978ROU/PER1 G. Roux, G. Perron, and J. E. Desnoyers, Can. J. Chem. **56**, 2808 (1978).
1978ROU/PER2 G. Roux, G. Perron, and J. E. Desnoyers, J. Solution Chem. **7**, 639 (1978).
1978RYB/EME V. I. Rybalkin, V. M. Emel'yanov, P. M. Stupak, N. R. Litovchenko, and M. I. Z'ola, Neftepererab. Neftekhim. (Kiev) **16**, 48 (1978).
1978SAF L. I. Safir, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **21**, 14 (1978).
1978SOL/SUK G. V. Solov'ev, G. I. Sukhinin, N. N. Stolyarov, and Yu. R. Chashkin, Kholod. Tekh. (6), 30 (1978).
1978STE W. V. Steele, J. Chem. Thermodyn. **10**, 919 (1978).
1978WOY/KAL M. Woycicka and B. Kalinowska, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **26**, 371 (1978).
1978ZHU/ATR I. P. Zhuk and T. R. Atrashenok, Inzh.-Fiz. Zh. **34**, 1027 (1978).
1979AMI/LEB E. B. Amitin, E. G. Lebedeva, and I. E. Paukov, Zh. Fiz. Khim. **53**, 2666 (1979).
1979AND/GRI R. A. Andolenko and B. A. Grigor'ev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **22**, 78 (1979).
1979BRO/ZIE G. N. Brown, Jr. and W. T. Ziegler, J. Chem. Eng. Data **24**, 319 (1979).
1979CZA I. Czarnota, Bull. Acad. Pol. Sci., Ser. Sci. Chim. **27**, 763 (1979).
1979DEV/SOM C. De Visser and G. Somsen, J. Solution Chem. **8**, 593 (1979).
1979DYK/REP J. Dykyj and M. Repáš, *Tlak nasytenej páry organických zlúčenin* (Veda, Bratislava, 1979).
1979DU/COM Du Pont 900 DTA, comercial calorimeter, Anal. Chim. Acta **27**, 763 (1979).
1979FOR/BEN J.-L. Fortier and G. C. Benson, J. Chem. Eng. Data **24**, 34 (1979).
1979FOR/DAR J.-L. Fortier, P. J. D'Arcy, and G. C. Benson, Thermochim. Acta **28**, 37 (1979).
1979FUC R. Fuchs, J. Chem. Thermodyn. **11**, 959 (1979).
1979GRI/YAN B. A. Grigor'ev, G. S. Yanin, and Yu. L. Rastorguev, Tr. GIAP **54**, 57 (1979).
1979GRO/HAM J.-P. E. Grolier, M. H. Hamedi, E. Wilhelm, and H. V. Kehiaian, Thermochim. Acta **31**, 79 (1979).
1979KIY/DAR O. Kiyohara, P. J. D'Arcy, and G. C. Benson, Can. J. Chem. **57**, 1006 (1979).
1979KOL K. Kollar-Hunek, Ph.D. thesis, Budapest Technical University, 1979.
1979MAR/BRA F. Martin Rubio, R. Bravo, M. Pintos, and A. Gomez-Gotor, Acta Cient. Compostelana **16**, 79 (1979).
1979MUR/SUB N. M. Murthy and S. V. Subrahmanyam, Indian J. Pure Appl. Phys. **17**, 620 (1979).
1979NIS/BAB V. P. Nistratov, A. G. Babinkov, K. G. Shvetsova, and S. A. Lapteva, Termodin. Org. Soedin. (8), 33 (1979).
1979OTT/GOA J. B. Ott, J. R. Goates, and R. B. Grigg, J. Chem. Thermodyn. **11**, 1167 (1979).
1979SAL/PEA P. P. S. Saluja, L. A. Peacock, and R. Fuchs, J. Am. Chem. Soc. **101**, 1958 (1979).
1979SCH/OFF R. C. F. Schaake, J. C. A. Offringa, G. J. K. Van der Berg, and J. C. Van Miltenburg, Recl. Trav. Chim. Pays-Bas **98**, 408 (1979).
1979SMI/GOO N. K. Smith and W. D. Good, AIAA J. **17**, 905 (1979).
1979STE W. V. Steele, J. Chem. Thermodyn. **11**, 1185 (1979).
1979STE/TAM M. A. Stephens and W. S. Tamplin, J. Chem. Eng. Data **24**, 81 (1979).
1979SVE C. Svensson, J. Chem. Thermodyn. **11**, 593 (1979).
1979TAK/YOK Y. Takahashi, H. Yokokawa, H. Kadokura, Y. Sekine, and T. Mukaibo, J. Chem. Thermodyn. **11**, 379 (1979).
1979VES/ZAB F. Veselý, M. Zábranský, V. Svoboda, and J. Pick, Collect. Czech. Chem. Commun. **44**, 3529 (1979).
1979WIL/FAR E. Wilhelm, A. Faradjzadeh, and J.-P. E. Grolier, J. Chem. Thermodyn. **11**, 979 (1979).
1979WIL/GRO E. Wilhelm, J.-P. E. Grolier, and M. H. Karbalai Ghassemi, Thermochim. Acta **28**, 59 (1979).
1980FUC R. Fuchs, Can. J. Chem. **58**, 2305 (1980).
1980GOO/THO W. D. Good, R. H. P. Thomas, B. E. Gammon, S. Lee-Bechtold, J. E. Callanan, and N. K. Smith, U.S. Deptartment of Energy Report, NIPER, Bartlesville No. 1, 1980 (unpublished).
1980KAL/JED B. Kalinowska, J. Jedlinska, W. Woycicki, and J. Stecki, J. Chem. Thermodyn. **12**, 891 (1980).
1980NAK/SUG N. Nakamura, H. Suga, and S. Seki, Bull. Chem. Soc. Jpn. **53**, 2755 (1980).

1980NEF/FIL S. N. Nefedov and L. P. Filippov, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **23**, 51 (1980).
1980ROU/ROB G. Roux, D. Roberts, G. Perron, and J. E. Desnoyers, J. Solution Chem. **9**, 629 (1980).
1980SHA/LYU R. F. Shakirov and M. V. Lyubarskii, deposited document SPSTL, 3Khp-D80, 1980.
1980VAS/TRE I. A. Vasil'ev, E. I. Treibsho, A. D. Korkhov, V. M. Petrov, N. G. Orlova, and M. M. Balakina, Inzh.-Fiz. Zh. **39**, 1054 (1980).
1981ARU G. S. Arutyunyan, Izv. Akad. Nauk Az. SSR, Ser. Fiz. -Tekn. Mat. Nauk **2**, 97 (1981).
1981ARU/BAG G. S. Arutyunyan, S. S. Bagdasaryan, and A. M. Kerimov, Izv. Akad. Nauk Az. SSR, Ser. Fiz. -Tekn. Mat. Nauk **2**, 94 (1981).
1981ATA/ELS S. R. Atalla, A. A. El-Sharkawy, and F. A. Gasser, Int. J. Thermophys. **2**, 155 (1981).
1981CAS/WIL C. Casanova, E. Wilhelm, J.-P. E. Grolier, and H. V. Kehiaian, J. Chem. Thermodyn. **13**, 241 (1981).
1981GRO/ING J.-P. E. Grolier, A. Inglese, A. H. Roux, and E. Wilhelm, Ber. Bunsenges. Phys. Chem. **85**, 768 (1981).
1981HOE G. W. H. Hoehne, Polym. Bull. (Berlin) **6**, 41 (1981).
1982BEN/DAR G. C. Benson and P. J. D'Arcy, J. Chem. Eng. Data **27**, 439 (1982).
1982BIR/SIK J. Biroš, A. Sikora, A. Živný, and J. Pouchlý, Collect. Czech. Chem. Commun. **47**, 2692 (1982).
1982GOR/SIM1 N. I. Gorbunova, V. M. Simonov, and V. A. Shipova, Dokl. Akad. Nauk SSSR **266**, 850 (1982).
1982GOR/SIM2 N. I. Gorbunova, V. M. Simonov, and V. A. Shipova, *Proceedings of the Eighth Symposium on Thermophysics Properties*, edited by J. V. Sengers (American Society of Mechanical Engineers, New York, 1982), p. 409.
1982GRO/ING J.-P. E. Grolier, A. Inglese, and E. Wilhelm, J. Chem. Thermodyn. **14**, 523 (1982).
1982LEB/BYK B. V. Lebedev, T. A. Bykova, N. N. Smirnova, and T. G. Kulagina, Zh. Obshch. Khim. **52**, 2630 (1982).
1982MAR/AND J. F. Martin and R. J. L. Andon, J. Chem. Thermodyn. **14**, 679 (1982).
1982OLL/PER M. Ollivon and R. Perron, Thermochim. Acta **53**, 183 (1982).
1982PFE/KUC R. Pfestorf, D. Kuchenbecker, and K. Quitzsch, Z. Phys. Chem. (Leipzig) **263**, 233 (1982).
1982TAN R. Tanaka, J. Chem. Thermodyn. **14**, 259 (1982).
1982VAS/PET I. A. Vasil'ev, V. M. Petrov, and E. I. Treibsho, Zh. Prikl. Khim. (Leningrad) **55**, 2116 (1982).
1982VIL/CAS M. A. Villamanan, C. Casanova, G. Roux-Desgranges, and J.-P. E. Grolier, Thermochim. Acta **52**, 279 (1982).
1982VOR/YAK A. F. Vorob'ev and P. N. Yakovlev, Zh. Fiz. Khim. **56**, 1933 (1982).
1982WIL/FAR E. Wilhelm, A. Faradjzadeh, and J.-P. E. Grolier, J. Chem. Thermodyn. **14**, 1199 (1982).
1982WIL/ING E. Wilhelm, A. Inglese, J. R. Quint, and J.-P. E. Grolier, J. Chem. Thermodyn. **14**, 303 (1982).
1982ZAR Z. I. Zaripov, Teplomasoobmen Teplofiz. Svoistva Veshchestv (Sb. Nauchnykh Trudov) 73 (1982).
1983BEN/DAR G. C. Benson, P. J. D'Arcy, and M. E. Sugamori, Thermochim. Acta **71**, 161 (1983).
1983BYK/LEB2 T. A. Bykova, B. V. Lebedev, and E. N. Tarasov, Termodin. Org. Soedin. 48 (1983).
1983DAP/DEL A. D'Aprano, R. DeLisi, and D. I. Donato, J. Solution Chem. **12**, 383 (1983).
1983DEK/VAN C. G. De Kruif, J. C. Van Miltenburg, and J. G. Blok, J. Chem. Thermodyn. **15**, 129 (1983).
1983GOR/SIM N. I. Gorbunova, V. M. Simonov, and V. A. Shipova, Teplofiz. Vys. Temp. **21**, 270 (1983).
1983GRO/FAR1 J.-P. E. Grolier and A. Faradjzadeh, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 250 (1983).
1983GRO/FAR2 J.-P. E. Grolier and A. Faradjzadeh, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 251 (1983).
1983GRO/FAR3 J.-P. E. Grolier and A. Faradjzadeh, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 252 (1983).
1983KUK/KOR V. A. Kukharenko, V. P. Korolev, and G. A. Krestov, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **26**, 369 (1983).
1983MCG J. McGarry, Ind. Eng. Chem. Prod. Res. Dev. **2**, 313 (1983).
1983MEY/MEY E. F. Meyer and M. C. Meyer, J. Chem. Eng. Data **28**, 148 (1983).
1983ORO/MRA D. F. O'Rourke and S. C. Mraw, J. Chem. Thermodyn. **15**, 489 (1983).
1983PFE/SCH R. Pfestorf, J. Schmelzer, M. Krug, B. Zeiger, U. Stych, and K. Quitzsch, Fluid Phase Equilib. **12**, 283 (1983).
1983ROU/ROU A. H. Roux, G. Roux-Desgranges, J.-P. E. Grolier, and A. Viallard, Calorim. Anal. Therm. **14**, 142 (1983).
1983SID/SVE M. A. Siddiqi, P. Svejda, and F. Kohler, Ber. Bunsenges. Phys. Chem. **87**, 1176 (1983).
1983TAK/KAD Y. Takahashi, H. Kadokura, and H. Yokokawa, J. Chem. Thermodyn. **15**, 65 (1983).
1983YOS/SOR1 M. Yoshikawa, M. Sorai, H. Suga, and S. Seki, J. Phys. Chem. Solids **44**, 311 (1983).
1984AMI/MIN E. B. Amitin, Yu. F. Minenkov, O. A. Nabutovskaya, I. E. Paukov, and S. I. Sokolova, J. Chem. Thermodyn. **16**, 431 (1984).
1984BEN/DAR G. C. Benson, P. J. D'Arcy, and M. K. Kumaran, Thermochim. Acta **75**, 353 (1984).
1984BRA/PIN R. Bravo, M. Pintos, M. C. Baluja, M. I. Paz Andrade, G. Roux-Desgranges, and J.-P. E. Grolier, J. Chem. Thermodyn. **16**, 73 (1984).
1984DYK/REP J. Dykyj, M. Repáš, and J. Svoboda, *Tlak nasytenej páry organických zlúčenin* (Veda, Bratislava, 1984).
1984FIL/LAU L. P. Filippov and L. A. Laushkina, Zh. Fiz. Khim. **58**, 1068 (1984).
1984GRI/AND B. A. Grigor'ev and R. A. Andolenko, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **27**, 60 (1984).
1984GRO/BEN J.-P. E. Grolier and G. C. Benson, Can. J. Chem. **62**, 949 (1984).
1984GRO/ING J.-P. E. Grolier, A. Inglese, and E. Wilhelm, J. Chem. Thermodyn. **16**, 67 (1984).
1984GUS/MIR S. O. Guseinov and A. A. Mirzaliev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **27**, 41 (1984).
1984ING/GRO A. Inglese, J.-P. E. Grolier, and E. Wilhelm, Fluid Phase Equilib. **15**, 287 (1984).
1984KAL/WOY B. Kalinowska and W. Woycicki, J. Chem. Thermodyn. **16**, 609 (1984).
1984KUM/BEN M. K. Kumaran, G. C. Benson, P. J. D'Arcy, and C. J. Halpin, J. Chem. Thermodyn. **16**, 1181 (1984).
1984ROU/GRO A. H. Roux, J.-P. E. Grolier, A. Inglese, and E. Wilhelm, Ber. Bunsenges. Phys. Chem. **88**, 986 (1984).
1984STE/OLS M. Stephens and J. D. Olson, Thermochim. Acta **76**, 79 (1984).
1984STO/CHA N. N. Stolyarov and Yu. R. Chashkin, Kholod. Tekh. (2), 39 (1984).
1984ZEG/SOM2 H. C. Zegers and G. Somsen, J. Chem. Thermodyn. **16**, 225 (1984).
1985BAL/BRA M. C. Baluja, R. Bravo, M. Pintos, M. I. Paz Andrade, G. Roux-Desgranges, and J.-P. E. Grolier, Calorim. Anal. Therm. **16**, 138 (1985).
1985BEN/KUM G. C. Benson, M. K. Kumaran, T. Treszczanowicz, P. J. D'Arcy, and C. J. Halpin, Thermochim. Acta **95**, 59 (1985).
1985CAM/THO S. W. Campbell and G. Thodos, J. Chem. Eng. Data **30**, 102 (1985).
1985COS/PAT1 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 212 (1985).
1985COS/PAT2 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 213 (1985).
1985COS/PAT3 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 214 (1985).
1985COS/PAT4 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 215 (1985).
1985COS/PAT5 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 216 (1985).
1985COS/PAT6 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 217 (1985).
1985COS/PAT7 M. Costas and D. Patterson, Int. Data Ser., Sel. Data Mix-

tures, Ser. A (3), 222 (1985).
1985COS/PAT8 M. Costas and D. Patterson, J. Chem. Soc., Faraday Trans. 1 **81**, 635 (1985).
1985COS/PAT9 M. Costas and D. Patterson, J. Chem. Soc., Faraday Trans. 1 **81**, 2381 (1985).
1985CZA I. Czarnota, High Temp. - High Press. **17**, 543 (1985).
1985GUS/DAV E. A. Gusev, S. V. Davidovich, and A. A. Vecher, Thermochim. Acta **92**, 379 (1985).
1985HEP/KOO L. G. Hepler, Z. S. Kooner, G. Roux-Desgranges, and J.-P. E. Grolier, J. Solution Chem. **14**, 579 (1985).
1985LAI/GRO A. Lainez, J.-P. E. Grolier, and E. Wilhelm, Thermochim. Acta **91**, 243 (1985).
1985LAI/ROD A. Lainez, M. Rodrigo, A. H. Roux, J.-P. E. Grolier, and E. Wilhelm, Calorim. Anal. Therm. **16**, 153 (1985).
1985LAI/ROU A. Lainez, G. Roux-Desgranges, J.-P. E. Grolier, and E. Wilhelm, Fluid Phase Equilib. **20**, 47 (1985).
1985LAI/WIL A. Lainez, E. Wilhelm, G. Roux-Desgranges, and J.-P. E. Grolier, J. Chem. Thermodyn. **17**, 1153 (1985).
1985NKI/CHA P. Nkinamubanzi, G. Charlet, and G. Delmas, Fluid Phase Equilib. **20**, 57 (1985).
1985OGA H. Ogawa and S. Murakami, Thermochim. Acta **88**, 255 (1985).
1985RAB/NOV I. B. Rabinovich, N. V. Novoselova, E. M. Moseeva, A. G. Babinkov, and L. Ya. Tsvetkova, Zh. Fiz. Khim. **59**, 2127 (1985).
1985RAB/SHE I. B. Rabinovich, M. S. Sheiman, V. P. Nistratov, G. P. Kamelova, and A. D. Zorin, Zh. Fiz. Khim. **59**, 2414 (1985).
1985TAN R. Tanaka, J. Chem. Eng. Data **30**, 267 (1985).
1985TAN/NAK R. Tanaka, T. Nakamichi, and S. Murakami, J. Solution Chem. **14**, 795 (1985).
1986BEN/DAR1 G. C. Benson and P. J. D'Arcy, Can. J. Chem. **64**, 2139 (1986).
1986BEN/DAR2 G. C. Benson and P. J. D'Arcy, J. Chem. Thermodyn. **18**, 493 (1986).
1986BEN/DAR3 G. C. Benson and P. J. D'Arcy, Thermochim. Acta **102**, 75 (1986).
1986BEN/KUM G. C. Benson, M. K. Kumaran, C. J. Halpin, and P. J. D'Arcy, J. Chem. Thermodyn. **18**, 1007 (1986).
1986DJO/LAU N. M. Djordjevic and R. J. Laub, Thermochim. Acta **107**, 227 (1986).
1986GAT/WOO J. A. Gates, R. H. Wood, J. C. Cobos, C. Casanova, A. H. Roux, G. Roux-Desgranges, and J.-P. E. Grolier, Fluid Phase Equilib. **27**, 137 (1986).
1986JIM/ROM E. Jimenez, L. Romani, M. I. Paz Andrade, G. Roux-Desgranges, and J.-P. E. Grolier, J. Solution Chem. **15**, 879 (1986).
1986KOR/KUK V. P. Korolev, V. A. Kukharenko, and G. A. Krestov, Zh. Fiz. Khim. **60**, 1854 (1986).
1986KRU/FED T. I. Kruchina, N. V. Fedyainov, V. A. Vasilev, and V. F. Nazimok, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **29**, 53 (1986).
1986MER/BEN J. Mercier, L. Benoist, and P. Le Parlouer, Journees d'Etude sur les Capac. Calor. des Syst. Condenses, Cadarache, France, 1986, p. 164.
1986NAZ/BAS1 Ya. M. Naziev, M. M. Bashirov, and Yu. A. Badalov, Inzh.-Fiz. Zh. **51**, 789 (1986).
1986NAZ/BAS2 Ya. M. Naziev, M. M. Bashirov, and Yu. A. Badalov, Inzh.-Fiz. Zh. **51**, 998 (1986).
1986NIL/WAD S.-O. Nilsson and I. Wadso, J. Chem. Thermodyn. **18**, 673 (1986).
1986NOV/RAB N. V. Novoselova, I. B. Rabinovich, L. Ya. Tsvetkova, E. M. Moseeva, and A. G. Babinkov, Zh. Fiz. Khim. **60**, 1627 (1986).
1986OGA/MUR H. Ogawa and S. Murakami, Thermochim. Acta **109**, 145 (1986).
1986ORT J. Ortega, Rev. Latinoam. Ing. Quim. Quim. Apl. (Lat. Am. J. Chem. Eng. Appl. Chem.) **16**, 307 (1986).
1986RAB/NOV I. B. Rabinovich, N. V. Novoselova, E. M. Moseeva, A. G. Babinkov, and L. Ya. Tsvetkova, Zh. Fiz. Khim. **60**, 545 (1986).
1986ROU/GRO G. Roux-Desgranges, J.-P. E. Grolier, M. A. Villamanan, and C. Casanova, Fluid Phase Equilib. **25**, 209 (1986).
1986SMI/SRI B. D. Smith and R. Srivastava, *Thermodynamic Data for Pure Compounds*, Physical Science Data 25, Part B (Elsevier, Amsterdam, 1986).
1986TAN/TOY R. Tanaka, S. Toyama, and S. Murakami, J. Chem. Thermodyn. **18**, 63 (1986).
1986WIL/LAI E. Wilhelm, A. Lainez, A. H. Roux, and J.-P. E. Grolier, Thermochim. Acta **105**, 101 (1986).
1987GRO/ROU J.-P. E. Grolier, G. Roux-Desgranges, Z. S. Kooner, J. F. Smith, and L. G. Hepler, J. Solution Chem. **16**, 745 (1987).
1987KAL/KOH H. Kalali, F. Kohler, and P. Svejda, Monatsch. Chem. **118**, 1 (1987).
1987LAN/CRI J. I. Lankford and C. M. Criss, J. Solution Chem. **16**, 885 (1987).
1987LES/LIC C. Lesbats and A. Lichanot, Thermochim. Acta **109**, 317 (1987).
1987MIR/SHA A. A. Mirzaliev, Sh. G. Shakhmuradov, and S. O. Guseinov, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **30**, 55 (1987).
1987NAZ/BAD Ya. M. Naziev, Yu. A. Badalov, and M. M. Bashirov, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **30**, 59 (1987).
1987OKH/RAZ V. S. Okhotin, L. A. Razumeichenko, and A. V. Skorodumov, Teplofiz. Vys. Temp. **25**, 812 (1987).
1987PER/COM Perkin-Elmer DSC-2C, commercial calorimeter, J. Chem. Eng. Data **32**, 251 (1987).
1987PIE H. Piekarski, Can. J. Chem. **65**, 2810 (1987).
1987SHV/PES O. V. Shvaro, A. D. Peshchenko, A. I. Sachek, V. G. Vasil'ev, and N. N. Smirnova, deposited document VINITI No. 1052-V87, 1987.
1987TAN R. Tanaka, J. Chem. Eng. Data **32**, 176 (1987).
1987VAN/VAN J. C. Van Miltenburg, J. K. Van den Berg, and M. J. Van Bommel, J. Chem. Thermodyn. **19**, 1129 (1987).
1987WIL/ING E. Wilhelm, A. Inglese, A. H. Roux, and J.-P. E. Grolier, Fluid Phase Equilib. **34**, 49 (1987).
1987WIL/LAI E. Wilhelm, A. Lainez, M. Berkane, G. Roux-Desgranges, A. H. Roux, and J.-P. E. Grolier, Calorim. Anal. Therm. **18**, 95 (1987).
1987YAM/OGU O. Yamamuro, M. Oguni, T. Matsuo, and H. Suga, Bull. Chem. Soc. Jpn. **60**, 1296 (1987).
1988AND/PAT L. Andreoli-Ball, D. Patterson, M. Costas, and M. Caceres-Alonso, J. Chem. Soc., Faraday Trans. 1 **84**, 3991 (1988).
1988ARU/MOV G. S. Arutyunyan and G. M. Movsesyan, Izv. Akad. Nauk Az. SSR, Ser. Fiz.-Tekn. Mat. Nauk **9**, 60 (1988).
1988BOY/CRI S. Boyette and C. M. Criss, J. Chem. Eng. Data **33**, 426 (1988).
1988CAC/COS M. Caceres-Alonso, M. Costas, L. Andreoli-Ball, and D. Patterson, Can. J. Chem. **66**, 989 (1988).
1988CON/GIA G. Conti, P. Gianni, A. Papini, and E. Matteoli, J. Solution Chem. **17**, 481 (1988).
1988COS/VAN M. Costas, H. Van Tra, D. Patterson, M. Caceros-Alonso, G. Tardajos, and E. Aicart, J. Chem. Soc., Faraday Trans. 1 **84**, 1603 (1988).
1988ING A. Inglese, Int. Data Ser., Sel. Data Mixtures, Ser. A (3), 170 (1988).
1988KOZ/KRA A. A. Kozyro, A. P. Krasulin, V. V. Simirskii, and V. S. Markovnik, Zh. Fiz. Khim. **62**, 1747 (1988).
1988KUZ/KHA M. A. Kuznetsov, V. E. Kharin, A. A. Gerasimov, and B. A. Grigor'ev, Izv. Vyssh. Ucheb. Zaved., Neft Gaz **31**, 49 (1988).
1988MEL/VER G. A. Mel'nikov, V. N. Verveiko, and N. F. Otpushchennikov, Zh. Fiz. Khim. **62**, 799 (1988).
1988MES/FIN J. F. Messerly, H. L. Finke, W. D. Good, and B. E. Gammon, J. Chem. Thermodyn. **20**, 485 (1988).
1988MUK/ZAR G. Kh. Mukhamedzyanov and Z. I. Zaripov, deposited document ONIITEKhIM (Cherkassy) N712-khp88, 1988, p. 1.
1988NAZ/BAS Ya. M. Naziev and M. M. Bashirov, Teplofiz. Vys. Temp. **26**, 58 (1988).
1988OKA/OGA T. Okano, H. Ogawa, and S. Murakami, Can. J. Chem. **66**, 713 (1988).
1988PER/AIC S. Perez-Casas, E. Aicart, L. M. Trejo, and M. Costas, Int.

Data Ser., Sel. Data Mixtures, Ser. A (2), 114 (1988).
1988PIE/SOM1 H. Piekarski and G. Somsen, J. Chem. Soc., Faraday Trans. **84**, 529 (1988).
1988PIE/SOM2 H. Piekarski and G. Somsen, Tenth IUPAC Conference on Chemical Thermodynamics, Prague, Czech Republic, 1988, Paper No. I-54.
1988PIN/BRA M. Pintos, R. Bravo, M. C. Baluja, M. I. Paz Andrade, G. Roux-Desgranges, and J.-P. E. Grolier, Can. J. Chem. **66**, 1179 (1988).
1988ROD/MAR F. Rodante and G. Marrosu, Thermochim. Acta **136**, 209 (1988).
1988SAI/TAN A. Saito and R. Tanaka, J. Chem. Thermodyn. **20**, 859 (1988).
1988SHI/OGA1 Y. Shiohama, H. Ogawa, S. Murakami, and I. Fujihara, J. Chem. Thermodyn. **20**, 1183 (1988).
1988SHI/OGA2 Y. Shiohama, H. Ogawa, S. Murakami, and I. Fujihara, J. Chem. Thermodyn. **20**, 1307 (1988).
1988STE/ARC W. V. Steele, D. G. Archer, R. D. Chirico, W. B. Collier, I. A. Hossenlopp, A. Nguyen, N. K. Smith, and B. E. Gammon, J. Chem. Thermodyn. **20**, 1233 (1988).
1988STE/CHI W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and N. K. Smith, NIPER Topical Report **395**, 1 (1988).
1989BAR/KOO1 L. Barta, Z. S. Kooner, L. G. Hepler, G. Roux-Desgranges, and J. P.-E. Grolier, J. Solution Chem. **18**, 663 (1989).
1989BAR/KOO2 L. Barta, Z. S. Kooner, L. G. Hepler, G. Roux-Desgranges, and J. P.-E. Grolier, Can. J. Chem. **67**, 1225 (1989).
1989BRE/LIC P. Bret-Dibat and A. Lichanot, Thermochim. Acta **147**, 261 (1989).
1989COB/GAR J. C. Cobos, I. Garcia, C. Casanova, G. Roux-Desgranges, and J.-P. E. Grolier, Int. Data Ser., Sel. Data Mixtures, Ser. A (1), 59 (1989).
1989DOU/KHA G. Douheret, A. Khadir, and A. Pal, Thermochim. Acta **142**, 219 (1989).
1989JIM/ROU E. Jimenez, G. Roux-Desgranges, J.-P. E. Grolier, and E. Wilhelm, Thermochim. Acta **151**, 99 (1989).
1989KNI/ARC S. E. Knipmeyer, D. G. Archer, R. D. Chirico, B. E. Gammon, I. A. Hossenlopp, A. Nguyen, N. K. Smith, W. V. Steele, and M. M. Strube, Fluid Phase Equilib. **52**, 185 (1989).
1989KOZ/MAR A. A. Kozyro, L. I. Marachuk, A. P. Krasulin, I. A. Yursha, and G. Ya. Kabo, Zh. Prikl. Khim. (Leningrad) **62**, 595 (1989).
1989KUL/KRE M. V. Kulikov, A. G. Krestov, L. P. Safonova, and A. M. Kolker, Termodinamika rastvorov neelektrolitov, Ivanovo, Russia, 1989, p. 27.
1989LAI/ROD A. Lainez, M.-M. Rodrigo, E. Wilhelm, and J.-P. E. Grolier, J. Chem. Eng. Data **34**, 332 (1989).
1989OHN/FUJ K. Ohnishi, I. Fujihara, and S. Murakami, Fluid Phase Equilib. **46**, 59 (1989).
1989PET/PES1 A. N. Petrov, P. B. Peshekhodov, and G. A. Al'per, Termodinam. Rastvorov Neelektrolitov, Ivanovo 21 (1989).
1989PFE/SCH R. Pfestorf, A. Schumichen, and K. Quitzsch, Z. Phys. Chem. (Leipzig) **270**, 1135 (1989).
1989PRA/RAJ T. E. V. Prasad, A. Rajiah, D. H. L. Prasad, and V. N. Swamy, Phys. Chem. Liq. **20**, 157 (1989).
1989SAI/SAT A. Saitoh, H. Sato, and K. Watanabe, Int. J. Thermophys. **10**, 649 (1989).
1989STE/CHI3 W. V. Steele, R. D. Chirico, A. Nguyen, I. A. Hossenlopp, and N. K. Smith, AIChE Symp. Ser. **85**, 140 (1989).
1989VES/BAR F. Veselý, P. Barcal, M. Zábranský, and V. Svoboda, Collect. Czech. Chem. Commun. **54**, 602 (1989).
1989VOG/SCH L. Vogel and H. Schuberth, Wiss. Z. Martin Luther Univ. Halle Wittenberg, Math. Naturwiss. Reihe **38**, 153 (1989).
1989WIL/LAI E. Wilhelm, A. Lainez, and J.-P. E. Grolier, Fluid Phase Equilib. **49**, 233 (1989).
1990CHI/GAM R. D. Chirico, B. E. Gammon, S. E. Knipmeyer, A. Nguyen, M. M. Strube, C. Tsonopoulos, and W. V. Steele, J. Chem. Thermodyn. **22**, 1075 (1990).
1990JAL/ROB D. Jalabert, J. B. Robert, and H. Roux-Buisson, Calorim. Anal. Therm. **20–21**, 441 (1990).
1990KOZ/SIM A. A. Kozyro, V. V. Simirkii, G. Ya. Kabo, M. L. Frenkel', A. P. Krasulin, V. M. Sebruk, and N. A. Sokolov, Zh. Fiz. Khim. **64**, 2360 (1990).
1990RAO/RAJ H. U. Rao, A. Rajiah, and D. H. L. Prasad, Indian Chem. Eng. **32**, 50 (1990).
1990SIN/GLI N. B. Singh and M. E. Glicksman, Thermochim. Acta **159**, 93 (1990).
1990SOR/ASA M. Sorai, S. Asahina, C. Destrade, and H. T. Nguyen, Liq. Cryst. **7**, 163 (1990).
1990TRE T. Treszczanowicz, Thermochim. Acta **160**, 253 (1990).
1990YAM/OGA K. Yamanaka, H. Ogawa, and S. Murakami, Thermochim. Acta **169**, 193 (1990).
1991ATR/NES T. R. Atrashenok, N. A. Nesterov, I. P. Zhuk, and A. D. Peshchenko, Inzh.-Fiz. Zh. **61**, 301 (1991).
1991BAN/GAR T. S. Banipal, S. K. Garg, and J. C. Ahluwalia, J. Chem. Thermodyn. **23**, 923 (1991).
1991BYK/KIP T. A. Bykova, E. G. Kiparisova, B. V. Lebedev, K. A. Mager, and Yu. G. Gololobov, Vysokomol. Soedin., Ser. A **33**, 614 (1991).
1991COB/GAR J. C. Cobos, I. Garcia, C. Casanova, A. H. Roux, G. Roux-Desgranges, and J.-P. E. Grolier, Fluid Phase Equilib. **69**, 223 (1991).
1991CZA I. Czarnota, J. Chem. Thermodyn. **23**, 25 (1991).
1991DES/PAT D. D. Deshpande, D. Patterson, L. Andreoli-Ball, M. Costas, and L. M. Trejo, J. Chem. Soc., Faraday Trans. **87**, 1133 (1991).
1991DOU/PAL G. Douheret, A. Pal, H. Hoiland, O. Anowi, and M. I. Davis, J. Chem. Thermodyn. **23**, 569 (1991).
1991DU/SUV Du Pont de Nemours, SUVA Refrigerants, Prospectus ER-8E, 1991.
1991GRO/ROU J.-P. E. Grolier, G. Roux-Desgranges, M. Berkane, and E. Wilhelm, J. Chem. Thermodyn. **23**, 421 (1991).
1991KAL/KOH H. Kalali, F. Kohler, and P. Svejda, J. Chem. Eng. Data **36**, 326 (1991).
1991KOZ/SHE A. A. Kozyro, M. S. Sheiman, G. Ya. Kabo, I. A. Yursha, and V. S. Kruk, Zh. Prikl. Khim. (Leningrad) **64**, 1704 (1991).
1991NAK S. Nakagawa, M.Sc. Thesis, Keio University, Japan, 1991.
1991OGA/MIT H. Ogawa, H. Mitsuo, H. Inoue, K. Tamura, and S. Murakami, Netsu Sokutei **18**, 150 (1991).
1991PES/NIK P. B. Peshekhodov, M. Yu. Nikiforov, G. A. Al'per, and G. A. Krestov, Zh. Obshch. Khim. **61**, 1535 (1991).
1991ROZ/SAF A. M. Rozhnov, V. V. Safronov, S. P. Verevkin, K. G. Sharonov, and V. I. Alenin, J. Chem. Thermodyn. **23**, 629 (1991).
1991SOE/NAK H. Soejima, H. Nakai, K. Tamura, H. Ogawa, and S. Murakami, Thermochim. Acta **177**, 305 (1991).
1991STE/CHI2 W. V. Steele, R. D. Chirico, A. Nguyen, I. A. Hossenlopp, and N. K. Smith, DIPPR Data Series (1991), 1 (Exp. Results Phase Equilib. Pure Compn. Prop.), 101-34.
1991SVO/ZAB1 V. Svoboda and M. Zábranský, Collect. Czech. Chem. Commun. **56**, 2786 (1991).
1991SVO/ZAB2 V. Svoboda, M. Zábranský, and M. Bárta, J. Chem. Thermodyn. **23**, 711 (1991).
1991TAN/ADA R. Tanaka and M. Adachi, J. Chem. Thermodyn. **23**, 1023 (1991).
1991TRE/COS L. M. Trejo, M. Costas, and D. Patterson, Int. Data Ser., Sel. Data Mixtures, Ser. A (1), 30 (1991).
1991VAS/LEB V. G. Vasilev and B. V. Lebedev, Vysokomol. Soedin., Ser. A **A33**, 818 (1991).
1991WIL/JIM E. Wilhelm, E. Jimenez, G. Roux-Desgranges, and J.-P. E. Grolier, J. Solution Chem. **20**, 17 (1991).
1992FIL/AFA V. A. Filatov and V. N. Afanas'ev, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **35(8)**, 97 (1992).
1992HWA/DES S. H. Hwang, D. D. DesMarteau, A. L. Beyerlein, N. D. Smith, and P. Joyner, J. Therm. Anal. **38**, 2515 (1992).
1992JAI/CHA D. V. S. Jain, R. Chadha, and S. K. Sehgal, Fluid Phase Equilib. **81**, 273 (1992).
1992KAB/KOZ G. J. Kabo, A. A. Kozyro, V. S. Krouk, V. M. Sevruk, I. A. Yursha, V. V. Simirsky, and V. I. Gogolinsky, J. Chem. Thermodyn. **24**, 1 (1992).
1992KAL/KOH H. Kalali, F. Kohler, and P. Svejda, J. Chem. Eng. Data **37**, 133 (1992).
1992KOL/KUL2 A. M. Kolker, M. V. Kulikov, and A. G. Krestov, Thermo-

chim. Acta **211**, 73 (1992).
1992LAI/ROD A. Lainez, M. M. Rodrigo, E. Wilhelm, and J.-P. E. Grolier, J. Solution Chem. **21**, 49 (1992).
1992MIY/TAM1 S. Miyanaga, K. Tamura, and S. Murakami, J. Chem. Thermodyn. **24**, 291 (1992).
1992MIY/TAM2 S. Miyanaga, K. Tamura, and S. Murakami, J. Therm. Anal. **38**, 1767 (1992).
1992NAZ/BAS Ya. M. Naziev, M. M. Bashirov, and M. A. Talybov, Zh. Prikl. Khim. (Leningrad) **65**, 2490 (1992).
1992PFE/SCH R. Pfestorf, A. Schumichen, and K. Quitzsch, Chem. Tech. (Leipzig) **44**, 140 (1992).
1992SIM/KOZ V. V. Simirskii, A. A. Kozyro, G. Ya. Kabo, J. A. Yurska, and L. I. Marachuk, Zh. Prikl. Khim. (Leningrad) **65**, 1638 (1992).
1992SOR/KAJ M. Sorai, K. Kaji, and Y. Kanebo, J. Chem. Thermodyn. **24**, 167 (1992).
1992VER/BEC S. P. Verevkin, H.-D. Beckhaus, and C. Ruechardt, Thermochim. Acta **197**, 27 (1992).
1993ANG/BOE C. A. Angell, L. Boehm, M. Oguni, and D. L. Smith, J. Mol. Liq. **56**, 275 (1993).
1993BAS/VOL M. Bastos, N. N. Volkova, and I. Wadso, J. Chem. Soc., Faraday Trans. **89**, 1351 (1993).
1993CHI/KNI2 R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and W. V. Steele, J. Chem. Thermodyn. **25**, 1461 (1993).
1993CON/GIR1 M. D. Contreras Claramonte, F. G. Vilchez, and A. P. Vialard, Thermochim. Acta **222**, 203 (1993).
1993CZA1 I. Czarnota, J. Chem. Thermodyn. **25**, 355 (1993).
1993CZA2 I. Czarnota, J. Chem. Thermodyn. **25**, 639 (1993).
1993DIK/KAB V. V. Diky, G. J. Kabo, A. A. Kozyro, A. P. Krasulin, and V. M. Sevruk, J. Chem. Thermodyn. **25**, 1169 (1993).
1993DU/SUV1 Du Pont de Nemours, SUVA Refrigerant HCFC-123, Prospectus T-123-SI, 1993.
1993DU/SUV2 Du Pont de Nemours, SUVA Refrigerant HCFC-124, Prospectus T-124-SI, 1993.
1993DUR/AOU N. Durupt, A. Aoulmi, M. Bouroukba, J. Jaubert, N. Neau, and M. Rogalski (private communication). Later equations published in Thermochim. Acta **260**, 87 (1995) and Thermochim. Acta **274**, 73 (1996).
1993FUJ/OGU1 H. Fujimori and M. Oguni, J. Phys. Chem. Solids **54**, 271 (1993).
1993GAR/BAN S. K. Garg, T. S. Banipal, and J. C. Ahluwalia, J. Chem. Thermodyn. **25**, 57 (1993).
1993GRO/ROU J.-P. E. Grolier, G. Roux-Desgranges, M. Berkane, E. Jimenez, and E. Wilhelm, J. Chem. Thermodyn. **25**, 41 (1993).
1993HAL D. Hallen, J. Chem. Thermodyn. **25**, 519 (1993).
1993KAP/BAL C. Kapseu, D. Balesdent, M. Dirand, and G. J. Kayem, J. Chim. Phys. Phys.-Chim. Biol. **90**, 457 (1993).
1993NAK/CHU M. Nakamura, K. Chubachi, K. Tamura, and S. Murakami, J. Chem. Thermodyn. **25**, 1311 (1993).
1993NAZ/BAS Ya. M. Naziev, M. M. Bashirov, M. A. Talybov, and Yu. A. Badalov, Teplofiz. Vys. Temp. **31**, 213 (1993).
1993PAG/HUO1 J.-Y. Page, M. Huot, and C. Jolicoeur, J. Chem. Thermodyn. **25**, 139 (1993).
1993SHE I. Shehatta, Thermochim. Acta **213**, 1 (1993).
1993STE/CHI2 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and I. R. Tasker, NIPER Topical Report **716**, 1 (1993).
1994BEN/ROU H. Bendiab, G. Roux-Desgranges, A. H Roux, J.-P. E. Grolier, and D. Patterson, J. Solution Chem. **23**, 307 (1994).
1994CHI/STE R. D. Chirico and W. V. Steele, Ind. Eng. Chem. Res. **33**, 157 (1994).
1994CON/GIA1 G. Conti, P. Gianni, and E. Matteoli, J. Chem. Thermodyn. **26**, 1249 (1994).
1994CON/GIA2 G. Conti, P. Gianni, and E. Matteoli, Thermochim. Acta **247**, 293 (1994).
1994FUJ/OGU H. Fujimori and M. Oguni, J. Chem. Thermodyn. **26**, 367 (1994).
1994GRO/ROU J.-P. E. Grolier, G. Roux-Desgranges, M. Berkane, and E. Wilhelm, J. Solution Chem. **23**, 153 (1994).
1994JIM/ROM E. Jimenez, L. Romani, E. Wilhelm, G. Roux-Desgranges, and J.-P. E. Grolier, J. Chem. Thermodyn. **26**, 817 (1994).
1994LAI/WIL A. Lainez, E. Wilhelm, and J.-P. E. Grolier, Monatsch. Chem. **125**, 877 (1994).
1994LEE L. L. Lee, Annual Report to Gas Research Institute, University of Oklahoma, 1994. From L.-F. Chiu, H.-F. Liu, and M.-H. Li, J. Chem. Eng. Data **44**, 631 (1999).
1994PRA/RAJ T. E. V. Prasad, A. Rajiah, and D. H. L. Prasad, Phys. Chem. Liq. **27**, 215 (1994).
1994SVO/CEJ V. Svoboda, D. Čejka, and M. Zábranský, J. Chem. Thermodyn. **26**, 147 (1994).
1995CON/GIA1 G. Conti, P. Gianni, L. Lepori, and E. Matteoli, Fluid Phase Equilib. **105**, 93 (1995).
1995CON/GIA2 G. Conti, P. Gianni, L. Lepori, and E. Matteoli, Fluid Phase Equilib. **108**, 255 (1995).
1995DIO/MAN H. P. Diogo, M. E. Manas de Piedade, J. A. M. Simoes, and Y. Nagano, J. Chem. Thermodyn. **27**, 597 (1995).
1995DUR/AOU N. Durupt, A. Aoulmi, M. Bouroukba, and M. Rogalski, Thermochim. Acta **260**, 87 (1995).
1995FUJ/TAM1 S. Fujii, K. Tamura, and S. Murakami, J. Chem. Thermodyn. **27**, 1319 (1995).
1995FUJ/TAM2 S. Fujii, K. Tamura, and S. Murakami, Thermochim. Acta **257**, 1 (1995).
1995KAB/KOZ1 G. J. Kabo, A. A. Kozyro, V. V. Diky, and V. V. Simirski, J. Chem. Eng. Data **40**, 371 (1995).
1995LAI/LOP A. Lainez, M. R. Lopez, M. Caceres, J. Munez, R. G. Rubio, J.-P. E. Grolier, and E. Wilhelm, J. Chem. Soc., Faraday Trans. **91**, 1941 (1995).
1995LEB/BYK1 B. V. Lebedev, T. A. Bykova, E. G. Kiparisova, B. G. Belenkaya, and V. N. Filatova, Vysokomol. Soedin., Ser. A Ser. B **37**, 187 (1995).
1995LOW/PEU B. Lowen, U. Peukert, and S. Schulz, Thermochim. Acta **255**, 1 (1995).
1995MOR/IDR1 N. A. Morad, M. Idrees, and A. A. Hasan, J. Therm. Anal. **44**, 823 (1995).
1995MOR/IDR2 N. A. Morad, M. Idrees, and A. A. Hasan, J. Therm. Anal. **45**, 1449 (1995).
1995NIS/OHO K. Nishikawa, K. Ohomuro, K. Tamura, and S. Murakami, Thermochim. Acta **267**, 323 (1995).
1995TAK/OGA T. Takigawa, H. Ogawa, M. Nakamura, K. Tamura, and S. Murakami, Fluid Phase Equilib. **110**, 267 (1995).
1995TAN/SUN Z. Tan, G. Sun, Y. Sun, A. Yin, W. Wang, J. Ye, and L. Zhou, J. Therm. Anal. **45**, 56 (1995).
1995WIL/ING E. Wilhelm, A. Inglese, A. Lainez, A. H. Roux, and J.-P. E. Grolier, Fluid Phase Equilib. **110**, 299 (1995).
1996GAL/VAN1 H. E. Gallis, G. J. K. Van den Berg, and H. A. J. Oonk, J. Chem. Eng. Data **41**, 1303 (1996).
1996KAB/BLO G. J. Kabo, A. V. Blokhin, A. A. Kozyro, and V. V. Diky, Thermochim. Acta **290**, 13 (1996).
1996LEB/SMI B. Lebedev, N. Smirnova, and V. Telnoy, Macromol. Chem. Phys. **197**, 3807 (1996).
1996LEB/VAS B. V. Lebedev, V. G. Vasilev, T. A. Bykova, E. G. Kiparisova, and B. Wunderlich, Vysokomol. Soedin., Ser. A Ser. B **38**, 216 (1996).
1996ROU/HER G. Roux-Desgranges, R. Herrmann, and J.-P. E. Grolier, ELDATA Int. J. Phys.-Chem. Data **2**, 185 (1996).
1996STE/CHI1 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **41**, 1255 (1996).
1996STE/CHI3 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and N. K. Smith, J. Chem. Eng. Data **41**, 1285 (1996).
1996TAN/TOY1 R. Tanaka and S. Toyama, J. Chem. Eng. Data **41**, 1455 (1996).
1996TAN/TOY2 R. Tanaka and S. Toyama, J. Chem. Thermodyn. **28**, 1403 (1996).
1996VAN/ALV J. C. van Miltenburg, A. Alvarez-Larena, M. Labrador, L. Palacios, J. Rodriguez-Romero, E. Tauler, and E. Estop, Thermochim. Acta **273**, 31 (1996).
1996ZAB/RUZ M. Zábranský, V. Růžička Jr., V. Majer, and E. S. Domalski, *Heat Capacity of Liquids. Critical Review and Recommended Values*, Monograph No. 6, (American Chemical Society, Washington DC, 1996), Vols. I and II.
1997ASA/SOR S. Asahina, M. Sorai, A. Fukuda, H. Takezoe, K. Furukawa, K. Terashima, Y. Suzuki, and I. Kawamura, Liq. Cryst. **23**, 339 (1997).
1997CEN/RUZ M. Čenský and K. Růžička, Calorimetry Experimental

Thermodynamics and Thermal Analysis Conference (CETTA'97), Zakopane, Poland, 1997, Paper No. C3, p. S5.
1997CHI/KNI2 R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and W. V. Steele, J. Chem. Eng. Data **42**, 248 (1997).
1997CHI/KNI3 R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and W. V. Steele, J. Chem. Eng. Data **42**, 772 (1997).
1997CHI/KNI4 R. D. Chirico, S. E. Knipmeyer, A. Nguyen, J. W. Reynolds, and W. V. Steele, J. Chem. Eng. Data **42**, 475 (1997).
1997COM/RIG F. Comelli, M. C. Righetti, and R. Francesconi, Thermochim. Acta **306**, 37 (1997).
1997CON/GIA G. Conti, P. Gianni, M. Tramati, L. Lepori, and E. Matteoli, J. Chem. Thermodyn. **29**, 865 (1997).
1997HOV/ROU S. Hovorka, A. H. Roux, G. Roux-Desgranges, and V. Dohnal, Calorimetry Experimental Thermodynamics and Thermal Analysis Conference (CETTA'97), Zakopane, Poland, 1997, Paper No. P30, p. S4.
1997HU/TAM1 J. Hu, K. Tamura, and S. Murakami, Fluid Phase Equilib. **131**, 197 (1997).
1997LEB/SMI B. V. Lebedev, N. N. Smirnova, and E. G. Kiparisova, Macromol. Chem. Phys. **198**, 41 (1997).
1997MAH/HEP Y. Maham, L. G. Hepler, A. E. Mather, A. W. Hakin, and R. A. Marriott, J. Chem. Soc., Faraday Trans. **93**, 1747 (1997).
1997NIS/TAB M. Nishimoto, S. Tabata, K. Tamura, and S. Murakami, Fluid Phase Equilib. **136**, 235 (1997).
1997RIG/COM M. C. Righetti, F. Comelli, and R. Francesconi, Thermochim. Acta **294**, 179 (1997).
1997STE/CHI2 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **42**, 1008 (1997).
1997STE/CHI3 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **42**, 1021 (1997).
1997STE/CHI4 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, A. Nguyen, and N. K. Smith, J. Chem. Eng. Data **42**, 1037 (1997).
1997SVO/GOT V. Svoboda, K. Gottmanová, V. Hynek, and B. Koutek, Collect. Czech. Chem. Commun. **62**, 1527 (1997).
1997TAN/NAK R. Tanaka and T. Nakamichi, J. Chem. Thermodyn. **29**, 221 (1997).
1997TAN/TOY R. Tanaka and S. Toyama, J. Chem. Eng. Data **42**, 871 (1997).
1997TOV/CAR1 C. A. Tovar, E. Carballo, C. A. Cerdeirina, M. I. Paz Andrade, and L. Romani, Fluid Phase Equilib. **136**, 223 (1997).
1997TOV/CAR3 C. A. Tovar, E. Carballo, C. A. Cardeirina, M. I. Paz Andrade, and L. Romani, J. Chem. Soc., Faraday Trans. **93**, 3505 (1997).
1997TOV/CAR4 C. A. Tovar, E. Carballo, C. A. Cerdeirina, J. L. Legido, and L. Romani, Int. J. Thermophys. **18**, 761 (1997).
1997VAR/DRU1 R. M. Varushchenko and A. I. Druzhinina, J. Chem. Thermodyn. **29**, 623 (1997).
1998ASA/SOR S. Asahina, M. Sorai, and R. Eidenschink, Liq. Cryst. **24**, 201 (1998).
1998BES/SAI D. Bessieres, H. Saint-Guirons, J. L. Daridon, P. Xans, and J.-Y. Coxam, J. Therm. Anal. **51**, 923 (1998).
1998CHI/COW R. D. Chirico, A. B. Cowell, W. D. Good, T. D. Klots, S. E. Knipmeyer, A. Nguyen, A. P. Rau, J. W. Reynolds, N. K. Smith, and W. V. Steele, J. Chem. Thermodyn. **30**, 1423 (1998).
1998CON/GIA G. Conti, P. Gianni, L. Lepori, and E. Matteoli, J. Chem. Thermodyn. **30**, 855 (1998).
1998HAW/GRA B. Hawrylak, K. Gracie, and R. Palepu, J. Solution Chem. **27**, 17 (1998).
1998HIK/OKA T. Hikima, N. Okamoto, M. Hanaya, and M. Oguni, J. Chem. Thermodyn. **30**, 509 (1998).
1998MUT/WIL M. L. Mutch and J. S. Wilkes, Proc.-Electrochem. Soc. **8**(11), 254 (1998).
1998ROH/MUS V. Roháč, J. E. Musgrove, K. Růžička, V. Růžička, M. Zábranský, and K. Aim, J. Chem. Thermodyn. **31**, 971 (1998).
1998RUZ/MAJ K. Růžička and V. Majer, 15th International Conference on Chemical Thermodynamics, Porto, Portugal, 1998, Paper No. C1-26.
1998SAL/FER G. Salvetti, C. Ferrari, and E. Tombari, Thermochim. Acta **316**, 47 (1998).
1998SOR/KIM M. Sorai, K. Kimura, A. Weiss, and R. Strauss, J. Chem. Thermodyn. **30**, 1441 (1998).
1998VAN/VAN J. C. van Miltenburg, A. C. G. van Genderen, and G. J. K. van den Berg, Thermochim. Acta **319**, 151 (1998).
1998VER2 S. P. Verevkin, Thermochim. Acta **316**, 131 (1998).
1998WIL/EGG E. Wilhelm, W. Egger, M. Vencour, A. H. Roux, M. Poledníček, and J.-P. E. Grolier, J. Chem. Thermodyn. **30**, 1509 (1998).
1998ZAM/ROG H. Zamali, J. Roger, C. Bergman, and J. C. Mathieu, Thermochim. Acta **311**, 37 (1998).
1999BRO/CAL1 P. Brocos, E. Calvo, R. Bravo, M. Pintos, A. Amigo, A. H. Roux, and G. Roux-Desgranges, J. Chem. Eng. Data **44**, 67 (1999).
1999BRO/CAL2 P. Brocos, E. Calvo, A. Pineiro, R. Bravo, A. Amigo, A. H. Roux, and G. Roux-Desgranges, J. Chem. Eng. Data **44**, 1341 (1999).
1999BUR/ZOC R. Burgdorf, A. Zocholl, W. Arlt, and H. Knapp, Fluid Phase Equilib. **164**, 225 (1999).
1999CAL/BRO E. Calvo, P. Brocos, A. Pineiro, M. Pintos, A. Amago, R. Bravo, A. H. Roux, and G. Roux-Desgranges, J. Chem. Eng. Data **44**, 948 (1999).
1999CER/TOV C. A. Cerdeirina, C. A. Tovar, J. Troncoso, E. Carballo, and L. Romani, Fluid Phase Equilib. **157**, 93 (1999).
1999CHI/LIU L.-F. Chiu, H.-F. Liu, and M.-H. Li, J. Chem. Eng. Data **44**, 631 (1999).
1999MO/YAN O. Mo, M. Yanez, M. V. Roux, P. Jimenez, J. Z. Davalos, M. A. V. Ribeiro da Silva, M. D. M. C. Ribeiro da Silva, M. A. R. M. Matos, L. M. P. F. Amaral, A. Sanches-Migallon, P Cabildo, R. Claramunt, J. Elguero, and J. F. Liebman, J. Phys. Chem. A **103**, 9336 (1999).
1999PAR/TOV J. M. Pardo, C. A. Tovar, C. A. Cardeirina, E. Carballo, and L. Romani, J. Chem. Thermodyn. **31**, 787 (1999).
1999PIN/BRA M. Pintos-Barral, R. Bravo, G. Roux-Desgranges, J.-P. E. Grolier, and E. Wilhelm, J. Chem. Thermodyn. **31**, 1151 (1999).
1999ROH/RUZ V. Roháč, V. Růžička, K. Růžička, M. Poledníček, K. Aim, J. Jose, and M. Zábranský, Fluid Phase Equilib. **57**, 121 (1999).
1999TAK/YAM K. Takeda, O. Yamamuro, I. Tsukushi, T. Matsuo, and H. Suga, J. Mol. Struct. **479**, 227 (1999).
1999TAM/OSA K. Tamura, A. Osaki, S. Murakami, H. Ohji, H. Ogawa, B. Laurent, and J.-P. E. Grolier, Fluid Phase Equilib. **156**, 137 (1999).
1999TAN/ZHA Z. C. Tan, J. B. Zhang, and S. H. Meng, J. Therm Anal. Calorim. **55**, 283 (1999).
1999VAN/OON J. C. van Miltenburg, H. A. J. Oonk, and V. Metivaud, J. Chem. Eng. Data **44**, 715 (1999).
1999VAN/TEN J. C. van Miltenburg and E. ten Grotenhuis, J. Chem. Eng. Data **44**, 721 (1999).
2000ATA/KAW T. Atake, H. Kawaji, T. Tojo, K. Kawasaki, Y. Ootsuka, M. Katou, and Y. Koga, Bull. Chem. Soc. Jpn. **73**, 1987 (2000).
2000BEC/AUF L. Becker, O. Aufderhaar, and J. Gmehling, J. Chem. Eng. Data **45**, 661 (2000).
2000BES/SAI1 D. Bessieres, H. Saint-Guirons, and J.-L. Daridon, J. Therm Anal. Calorim. **62**, 621 (2000).
2000BES/SAI2 D. Bessieres, H. Saint-Guirons, J.-L. Daridon, and J.-Y. Coxam, Meas. Sci. Technol. **11**, N69 (2000).
2000BLO/KAB A. V. Blokhin, G. Y. Kabo, and A. G. Kabo, Zh. Fiz. Khim. **74**, 989 (2000).
2000CDA CDATA, A Databank of Physicochemical Properties, Institute of Chemical Technology, Prague, 2000.
2000CER/MIG C. A. Cerdeirina, J. A. Miguez, E. Carballo, C. A. Tovar, E. de la Puente, and L. Romani, Thermochim. Acta **347**, 37 (2000).
2000DI/TAN1 Y. Y. Di, Z. C. Tan, Z. N. Li, Y. J. Song, Y. Zheng, S. H. Meng, and S. S. Qu, Thermochim. Acta **362**, 7 (2000).
2000DRU/VAR A. J. Druzhinina, R. M. Varuschenko, V. S. Sakrisova, and

A. A. Pimerzin, Zh. Fiz. Khim. **74**, 404 (2000).
2000ERN/CHO S. Ernst, M. Chorazewski, M. Tkaczyk, and P. Goralski, Fluid Phase Equilib. **174**, 33 (2000).
2000FUL/RUZ M. Fulem, K. Růžička, and V. Růžička, 14th International Congress on Chemical Process Engineering, CHISA 2000, Praha, Czech Republic, 2000, Paper no. C4.1.
2000MAG J. W. Magee, Int. J. Thermophys. **21**, 1303 (2000).
2000MAG/DUA J. W. Magee and H. A. Duarte-Garza, Int. J. Thermophys. **21**, 1351 (2000).
2000MOR/KAM N. A. Morad, A. A. M. Kamal, F. Panau, and T. W. Yew, J. Am. Oil Chem. Soc. **77**, 1001 (2000).
2000PAL/SZA M. Palczewska-Tulinska and A. M. Szafranski, J. Chem. Eng. Data **45**, 988 (2000).
2000ROH V. Roháč, Ph.D. thesis, Institute of Chemical Technology, 2000.
2000TAK/TAM T. Takigawa, K. Tamura, H. Ogawa, S. Murakami, and S. Takagi, Thermochim. Acta **352–353**, 25 (2000).
2000TAM/OSA K. Tamura and A. Osaki, Thermochim. Acta **352–353**, 11 (2000).
2000TOV/CER C. A. Tovar, C. A. Cerdeirina, D. Gonzales, E. Carballo, and L. Romani, Fluid Phase Equilib. **169**, 209 (2000).
2000URY/KUP V. F. Urďyash, V. F. Kupriyanov, N. Yu. Kokurina, A. G. Smirnov, and T. M. Kuleshova, Zh. Obshch. Khim. **70**, 719 (2000).
2000VAN J. C. van Miltenburg, Thermochim. Acta **343**, 57 (2000).
2001ASA/SOR S. Asahina and M. Sorai, Liq. Cryst. **28**, 1085 (2001).
2001BAL/MAT S. Baluja, T. Matsuo, and K. Tamura, J. Chem. Thermodyn. **33**, 1545 (2001).
2001BEC/GME L. Becker and J. Gmehling, J. Chem. Eng. Data **46**, 1638 (2001).
2001BES/SAI D. Bessieres, H. Saint-Guirons, and J.-L. Daridon, Phys. Chem. Liq. **39**, 301 (2001).
2001BYK/LEB T. A. Bykova, B. V. Lebedev, M. V. Ryabko, O. B. Gorbatsevich, and A. M. Muzafarov, Zh. Fiz. Khim. **75**, 604 (2001).
2001CER/TOV1 C. A. Cerdeirina, C. A. Tovar, D. Gonzales, E. Carballo, and L. Romani, Fluid Phase Equilib. **179**, 101 (2001).
2001CER/TOV2 C. A. Cerdeirina, C. A. Tovar, D. Gonzales-Salgado, E. Carballo, and L. Romani, Phys. Chem. Chem. Phys. **3**, 5230 (2001).
2001CHE/LI Y.-J. Chen and M.-H. Li, J. Chem. Eng. Data **46**, 102 (2001).
2001CHE/SHI Y.-J. Chen, T.-W. Shih, and M.-H. Li, J. Chem. Eng. Data **46**, 51 (2001).
2001DI/LI Y. Y. Di, Z. N. Li, S. H. Meng, Z. C. Tan, and S. S. Qu, Thermochim. Acta **373**, 31 (2001).
2001DI/SUN1 Y. Y. Di, X. H. Sun, Y. F. Liu, Z. C. Tan, S. H. Meng, S. L. Gao, and S. S. Qu, Huaxue Xuebao **59**, 496 (2001).
2001DI/SUN2 Y. Y. Di, X. H. Sun, Z. C. Tan, Y. F. Liu, S. H. Meng, S. L. Gao, and S. S. Qu, Thermochim. Acta **369**, 25 (2001).
2001KOZ/BLO A. A. Kozyro, A. V. Blokhin, G. J. Kabo, and Y. U. Paulechka, J. Chem. Thermodyn. **33**, 305 (2001).
2001LEB/SMI B. V. Lebedev, N. N. Smirnova, L. Y. Tsvetkova, and V. S. Iorish, J. Chem. Thermodyn. **33**, 389 (2001).
2001NGE/MAL S. P. Ngeyi, I. Malik, B. H. Justice, and E. F. Westrum, Jr., J. Chem. Thermodyn. **33**, 423 (2001).
2001PAR/TOV1 J. M. Pardo, C. A. Tovar, C. A. Cerdeirina, E. Carballo, and L. Romani, Fluid Phase Equilib. **179**, 151 (2001).
2001PEL/GON J. Peleteiro, D. Gonzales-Salgado, C. A. Cerdeirina, J. L. Valencia, and L. Romani, Fluid Phase Equilib. **191**, 83 (2001).
2001PAR/TOV2 J. M. Pardo, C. A. Tovar, D. Gonzales, E. Carballo, and L. Romani, J. Chem. Eng. Data **46**, 212 (2001).
2001SHE/KAR V. M. Sheiman, N. V. Karyakin, G. P. Kamelova, and B. J. Kozyrkin, Zh. Fiz. Khim. **75**, 1566 (2001).
2001SMI/LEB N. N. Smirnova and B. V. Lebedev, Russ. J. Phys. Chem. **75**, S118 (2001).
2001TAM K. Tamura, Fluid Phase Equilib. **182**, 303 (2001).
2001TAN/XUE Z. C. Tan, B. Xue, S. W. Lu, S. H. Meng, X. H. Yuan, and Y. J. Song, J. Therm Anal. Calorim. **63**, 297 (2001).
2001VAN/OON1 J. C. van Miltenburg, H. A. J. Oonk, and G. J. K. van den Berg, J. Chem. Eng. Data **46**, 84 (2001).
2001VAN/OON2 J. C. van Miltenburg, H. A. J. Oonk, and L. Ventola, J. Chem. Eng. Data **46**, 90 (2001).
2001VAR/DRU R. M. Varushchenko, A. J. Druyhinina, A. Yu. Churkina, and C.-T. Zhi, Zh. Fiz. Khim. **75**, 1351 (2001).
2001ZAB/RUZ M. Zábranský, V. Růžička, Jr., and E. S. Domalski, J. Phys. Chem. Ref. Data **30**, 1199 (2001).
2002BLO/PAU A. V. Blokhin, Y. U. Paulechka, G. J. Kabo, and A. A. Kozyro, J. Chem. Thermodyn. **34**, 29 (2002).
2002BRO/PIN P. Brocos, A. Pineiro, R. Bravo, A. Amigo, A. H. Roux, and G. Roux-Desgranges, J. Chem. Eng. Data **47**, 351 (2002).
2002CER/TOV C. A. Cerdeirina, C. A. Tovar, E. Carballo, L. Romani, M. del, C. Delgado, L. A. Torres, and M. Costas, J. Phys. Chem. B **106**, 185 (2002).
2002CHA/BLO M. B. Charapennikau, A. V. Blokhin, G. J. Kabo, A. G. Kabo, V. V. Diky, and A. G. Gusakov, Thermochim. Acta **382**, 109 (2002).
2002CHI/HIL J. S. Chickos, D. Hillesheim, G. Nichols, and M. J. Zehe, J. Chem. Thermodyn. **34**, 1647 (2002).
2002CHI/KNI1 R. D. Chirico, S. E. Knipmeyer, and W. V. Steele, J. Chem. Thermodyn. **34**, 1873 (2002).
2002CHI/KNI2 R. D. Chirico, S. E. Knipmeyer, and W. V. Steele, J. Chem. Thermodyn. **34**, 1885 (2002).
2002GON/TOV D. Gonzales-Salgado, C. A. Tovar, C. A. Cerdeirina, E. Carballo, and L. Romani, Fluid Phase Equilib. **199**, 121 (2002).
2002GOR/WAS P. Goralski, M. Wasiak, and A. Bald, J. Chem. Eng. Data **47**, 83 (2002).
2002HAN/HIK M. Hanaya, T. Hikima, M. Hatase, and M. Oguni, J. Chem. Thermodyn. **34**, 1173 (2002).
2002KAR/SHE N. V. Karyakin, M. S. Sheiman, M. S. Kozlova, G. P. Kamelova, V. N. Larina, and A. S. Smirnov, Zh. Fiz. Khim. **76**, 1186 (2002).
2002KOZ/KAR M. S. Kozlova, N. V. Karyakin, M. S. Sheiman, G. P. Kamelova, and V. N. Larina, Zh. Fiz. Khim. **76**, 1193 (2002).
2002LEB/BYK B. V. Lebedev, T. A. Bykova, A. V. Markin, A. R. Korigodskii, V. V. Kireev, and N. N. Sanina, Vysokomol. Soedin. Ser. A **44**, 2189 (2002).
2002LEB/VER B. Lebedev, V. Veridusova, H. Hocker, and H. Keul, Macromol. Chem. Phys. **203**, 1114 (2002).
2002LIP/SCH M. Lipovská, H. G. Schmidt, V. Roháč, V. Růžička, G. Wolf, and M. Zábranský, J. Therm Anal. Calorim. **68**, 753 (2002).
2002NAN/LIU Z. Nan, B. Liu, and Z. Tan, J. Chem. Thermodyn. **34**, 915 (2002).
2002PAR/GON J. M. Pardo, D. Gonzales-Salgado, C. A. Tovar, C. A. Cerdeirina, E. Carballo, and L. Romani, Can. J. Chem. **80**, 370 (2002).
2002PAR/ZOU R. Paramo, M. Zouine, and C. Casanova, J. Chem. Eng. Data **47**, 441 (2002).
2002PEL/GON J. Peleteiro, D. Gonzales-Salgado, C. A. Cerdeirina, and L. Romani, J. Chem. Thermodyn. **34**, 485 (2002).
2002ROH/FUL V. Roháč, M. Fulem, H.-G. Schmidt, V. Růžička, K. Růžička, and G. Wolf, J. Therm Anal. Calorim. **70**, 455 (2002).
2002SHE/KAR1 V. M. Sheiman, N. V. Karyakin, B. I. Kozyrkin, and J. A. Zelyaev, Zh. Fiz. Khim. **76**, 996 (2002).
2002SHE/KAR2 V. M. Sheiman, N. V. Karyakin, M. S. Sheiman, and I. A. Zelyaev, Russ. J. Phys. Chem. **76**, 881 (2002).
2002STE/CHI1 W. V. Steele, R. D. Chirico, A. B. Cowell, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 667 (2002).
2002STE/CHI2 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 648 (2002).
2002STE/CHI3 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 689 (2002).
2002STE/CHI4 W. V. Steele, R. D. Chirico, A. B. Cowell, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 700 (2002).
2002STE/CHI5 W. V. Steele, R. D. Chirico, A. B. Cowell, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 725 (2002).
2002STE/CHI6 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Eng. Data **47**, 715 (2002).
2002TAN/SUN Z. C. Tan, L. X. Sun, S. H. Meng, L. Li, F. Fu, P. Yu, B. P.

Liu, and J. B. Zhang, J. Chem. Thermodyn. **34**, 1417 (2002).
2002TSV/KUL L. J. Tsvetkova, T. G. Kulagina, and B. V. Lebedev, Vysokomol. Soedin., Ser. A Ser. B **44**, 474 (2002).
2002VAN/VAN1 J. C. van Miltenburg, G. J. K. van den Berg, and A. C. G. van Genderen, Thermochim. Acta **383**, 13 (2002).
2002VAN/VAN2 J. C. van Miltenburg and P. J. van Ekeren, Thermochim. Acta **385**, 11 (2002).
2002VAR/DRU R. M. Varushchenko and A. I. Druzhinina, Fluid Phase Equilib. **199**, 109 (2002).
2002ZHA/HAW K. Zhang, B. Hawrylak, R. Palepu, and P. R. Tremaine, J. Chem. Thermodyn. **34**, 679 (2002).
2003ASA/SOR S. Asahina and M. Sorai, J. Chem. Thermodyn. **35**, 649 (2003).
2003BRO/PIN1 P. Brocos, A. Pineiro, R. Bravo, A. Amigo, A. H. Roux, and G. Roux-Desgranges, J. Chem. Eng. Data **48**, 712 (2003).
2003BRO/PIN2 P. Brocos, A. Pineiro, R. Bravo, A. Amigo, A. H. Roux, and G. Roux-Desgrandes, J. Chem. Eng. Data **48**, 1055 (2003).
2003CEN/RUZ M. Čenský, K. Růžička, V. Růžička, and M. Zábranský, Thermochim. Acta **93**, 45 (2003).
2003CHA/BLO M. B. Charapennikau, A. V. Blokhin, A. G. Kabo, and G. J. Kabo, J. Chem. Thermodyn. **35**, 145 (2003).
2003CHI/KNI R. D. Chirico, S. E. Knipmeyer, and W. V. Steele, J. Chem. Thermodyn. **35**, 1059 (2003).
2003GOR/TKA P. Goralski, M. Tkaczyk, and M. Chorazewski, J. Chem. Eng. Data **48**, 492 (2003).
2003HOL/REI J. D. Holbrey, W. M. Reichert, R. G. Reddy, and R. D. Rogers, ACS Symp. Ser. **856**, 121 (2003).
2003KON/TAN L.-G. Kong, Z.-C. Tan, J. Xu, S.-H. Meng, and X.-H. Bao, J. Chem. Thermodyn. **35**, 1897 (2003).
2003KOZ/KAR M. S. Kozlova, N. V. Karyakin, M. S. Sheiman, G. P. Kamelova, V. N. Larina, and A. S. Smirnov, Zh. Fiz. Khim. **77**, 30 (2003).
2003PAR/ZOU R. Paramo, M. Zouine, F. Sobron, and C. Casanova, Int. J. Thermophys. **24**, 185 (2003).
2003ROJ/ORO A. Rojas and E. Orozco, Thermochim. Acta **405**, 93 (2003).
2003STE/CHI W. V. Steele, R. D. Chirico, A. B. Cowell, A. Nguyen, and S. E. Knipmeyer, J. Chem. Thermodyn. **35**, 1253 (2003).
2003VAN/GAB J. C. van Miltenburg, H. Gabrielová, and K. Růžička, J. Chem. Eng. Data **48**, 1323 (2003).
2003VAN/VAN1 J. C. van Miltenburg, G. J. K. van den Berg, and M. Ramirez, J. Chem. Eng. Data **48**, 36 (2003).
2003VAN/VAN2 J. C. van Miltenburg, P. J. van Ekeren, F. G. Gandolfo, and E. Floeter, J. Chem. Eng. Data **48**, 1245 (2003).
2003YAN/MA1 C. Yang, P. Ma, F. Jing, and D. Tang, J. Chem. Eng. Data **48**, 836 (2003).
2003YAN/MA2 C. Yang, P. Ma, and S. Xia, Tianjin Daxue Xuebao (J. Tianjin University) **36**, 192 (2003).
2004BLO/KAB A. V. Blokhin, A. G. Kabo, M. P. Shymanovich, A. B. Bazyleva, and M. B. Charapennikau, Vestsi Nats. Akad. Navuk Belarusi, Ser. Khim. Navuk (3), 47 (2004).
2004BOL/NER M. F. Bolotnikov and Yu. A. Neruchev, J. Chem. Eng. Data **49**, 202 (2004).
2004BRO/PIN P. Brocos, A. Pineiro, R. Bravo, A. Amigo, A. H. Roux, and G. Roux-Desgrandes, J. Chem. Eng. Data **49**, 647 (2004).
2004BYK/LEB T. A. Bykova and B. V. Lebedev, Russ. J. Gen. Chem. **74**, 250 (2004).
2004BYK/SMI T. A. Bykova, N. N. Smirnova, L. V. Nikishchenkova, G. P. Belov, and E. V. Novikova, Zh. Fiz. Khim. **78**, 1944 (2004).
2004CER/GON C. A. Cerdeiriña, D. Gonzáles-Salgado, L. Romani, M. C. Delgado, L. A. Torres, and M. Costas, J. Chem. Phys. **120**, 6648 (2004).
2004CHE/CLE Y. Chernyak and J. H. Clements, J. Chem. Eng. Data **49**, 1180 (2004).
2004CHI/STE R. D. Chirico and W. V. Steele, J. Chem. Thermodyn. **36**, 633 (2004).
2004DI/TAN Y. Y. Di, Z. C. Tan, X. H. Sun, M. H. Wang, F. Xu, Y. F. Liu, L. X. Sun, and H. T. Zhang, J. Chem. Thermodyn. **36**, 79 (2004).
2004DIN M. S. Ding, J. Chem. Eng. Data **49**, 276 (2004).
2004DRU/VAR A. I. Druzhinina, R. M. Varushchenko, E. L. Krasnykh, and S. V. Levanova, Zh. Fiz. Khim. **78**, 2161 (2004).
2004FEN/PER D. Fenclová, S. Perez-Casas, M. Costas, and V. Dohnal, J. Chem. Eng. Data **49**, 1833 (2004).
2004FRE/CRO C. P. Fredlake, J. M. Crosthwaite, D. G. Hert, S. N. V. K. Aki, and J. F. Brennecke, J. Chem. Eng. Data **49**, 954 (2004).
2004GON/PEL D. Gonzales-Salgado, J. Peleteiro, J. Troncoso, E. Carballo, and L. Romani, J. Chem. Eng. Data **49**, 333 (2004).
2004KAB/BLO G. J. Kabo, A. V. Blokhin, Y. V. Paulechka, A. G. Kabo, and M. P. Shymanovich, J. Chem. Eng. Data **49**, 453 (2004).
2004KIM/SHI K.-S. Kim, B.-K. Shin, H. Lee, and F. Ziegler, Fluid Phase Equilib. **218**, 215 (2004).
2004LV/TAN X. C. Lv, Z. C. Tan, Y. Y. Di, Q. She, L. X. Sun, and T. Zhang, J. Chem. Thermodyn. **36**, 787 (2004).
2004MAS/NAK M. Massalska-Arodz, T. Nakamoto, T. Wasiutynski, J. Mayer, J. Krawczyk, and M. Sorai, J. Chem. Thermodyn. **36**, 877 (2004).
2004NAN/TAN Z. D. Nan and Z. C. Tan, J. Therm Anal. Calorim. **76**, 955 (2004).
2004PAR/ZOU R. Paramo, M. Zouine, F. Sobron, and C. Casanova, J. Chem. Eng. Data **49**, 58 (2004).
2004PAU/ZAI Y. U. Paulechka, D. H. Zaitsau, and G. J. Kabo, Hydrocarbon Process., Int. Ed. **115**, 105 (2004).
2004PEL/TRO J. Peleteiro, J. Troncoso, D. Gonzales-Salgado, J. L. Valencia, C. A. Cerdeirina, and L. Romani, Int. J. Thermophys. **25**, 787 (2004).
2004REB/NAJ L. P. N. Rebelo, V. Najdanovic-Visak, Z. P. Visak, M. Nunes da Ponte, J. Szydlowski, C. A. Cerdeirina, J. Troncoso, and L. Romani, Green Chem. **6**, 369 (2004).
2004RUZ/FUL K. Růžička, M. Fulem, and V. Růžička, Thermochim. Acta **421**, 35 (2004).
2004RYA/LEB M. V. Ryabkov, B. V. Lebedev, N. N. Smirnova, E. V. Agina, S. A. Ponomarenko, E. A. Makeev, N. I. Boiko, and V. P. Shibaev, Zh. Fiz. Khim. **78**, 1950 (2004).
2004SMI/MAR N. N. Smirnova, A. V. Markin, K. V. Kandeev, H. Hocker, and H. Keul, Thermochim. Acta **409**, 55 (2004).
2004STE/CHI1 W. V. Steele, R. D. Chirico, A. B. Cowell, A. Nguyen, and S. E. Knipmeyer, J. Chem. Thermodyn. **36**, 497 (2004).
2004STE/CHI2 W. V. Steele, R. D. Chirico, S. E. Knipmeyer, and A. Nguyen, J. Chem. Thermodyn. **36**, 845 (2004).
2004SUN/LIU X.-H. Sun, Y.-F. Liu, Z.-C. Tan, Y.-Y. Di, H.-F. Wang, and M.-H. Wang, J. Chem. Thermodyn. **36**, 895 (2004).
2004SUN/SON X.-H. Sun, J.-R. Song, Z.-C. Tan, Y.-Y. Di, H.-X. Ma, M.-H. Wang, and L.-X. Sun, Thermochim. Acta **413**, 261 (2004).
2004TRO/VAL J. Troncoso, J. L. Valencia, M. Sonto-Caride, D. Gonzales-Salgado, and J. Peleteiro, J. Chem. Eng. Data **49**, 1789 (2004).
2004VAN/OON M. J. van Bommel, H. A. J. Oonk, and J. C. van Miltenburg, J. Chem. Eng. Data **49**, 1036 (2004).
2004VAN/VAN J. C. van Miltenburg and G. J. K. van den Berg, J. Chem. Eng. Data **49**, 735 (2004).
2004WAN/TAN1 M.-H. Wang, Z.-C. Tan, X.-H. Sun, F. Xu, Y.-F. Liu, L.-X. Sun, and T. Zhang, Thermochim. Acta **414**, 25 (2004).
2004WAN/TAN2 S.-X. Wang, Z.-C. Tan, Y.-Y. Di, F. Xu, H.-T. Zhang, L.-X. Sun, and T. Zhang, J. Chem. Thermodyn. **36**, 393 (2004).
2004WAN/TAN3 M.-H. Wang, Z.-C. Tan, X.-H. Sun, Y.-F. Liu, H.-F. Wang, L.-X. Sun, and T. Zhang, J. Chem. Thermodyn. **36**, 477 (2004).
2004WAN/TAN4 M.-H. Wang, Z.-C. Tan, X.-H. Sun, F. Xu, L.-G. Kong, L.-X. Sun, and T. Zhang, Thermochim. Acta **411**, 203 (2004).
2004XU/SUN F. Xu, L.-X. Sun, Z.-C. Tan, J.-G. Liang, and R.-L. Li, Thermochim. Acta **412**, 33 (2004).
2004XUE/WAN B. Xue, J.-Y. Wang, Z.-C. Tan, S.-W. Lu, and S.-M. Meng, J. Therm Anal. Calorim. **76**, 965 (2004).
2004YAN/MA C. Yang, P. Ma, and Q. Zhou, J. Chem. Eng. Data **49**, 582

(2004).
2004ZAI/PAV D. G. Zaitsev, E. V. Pavlechko, G. Ya. Kabo, A. V. Blokhin, T. S. Kjasanshin, and O. G. Poddubskii, Vestsi Nats. Akad. Navuk Belarusi, Ser. Khim. Navuk No. 1, 66 92004).
2004ZOU/TAN G.-L. Zou, Z.-C. Tan, Y.-Y. Di, X.-Z. Lan, L.-X. Sun, and T. Zhang, Thermochim. Acta **423**, 83 (2004).
2005BAZ/BLO A. B. Bazyleva, A. V. Blokhin, G. J. Kabo, A. G. Kabo, and Y. U. Paulechka, J. Chem. Thermodyn. **37**, 643 (2005).
2005BYK/NIK T. A. Bykova, L. V. Nikishchenkova, N. N. Smirnova, G. P. Belov, and E. V. Novikova, Russ. J. Phys. Chem. **79**, 862 (2005).
2005CHI/STE1 R. D. Chirico and W. V. Steele, J. Chem. Eng. Data **50**, 697 (2005).
2005CHI/STE2 R. D. Chirico and W. V. Steele, J. Chem. Eng. Data **50**, 1052 (2005).
2005CHO/GOR M. Chorazewski, P. Goralski, and M. Tkaczyk, J. Chem. Eng. Data **50**, 619 (2005).
2005CRO/MUL J. M. Crosthwaite, M. J. Muldoon, J. N. K. Dixon, J. L. Anderson, and J. F. Brennecke, J. Chem. Thermodyn. **37**, 559 (2005).
2005DOM/BOG U. Domanska and R. Bogel-Lukasik, J. Phys. Chem. B **109**, 12124 (2005).
2005DOM/MAR U. Domanska and M. Marciniak, Fluid Phase Equilib. **235**, 30 (2005).
2005FRA/BIG R. Francesconi, A. Bigi, K. Rubini, and F. Comelli, J. Chem. Eng. Data **50**, 1932 (2005).
2005FUJ/MAT M. Fujisawa, T. Matsushita, and T. Kimura, J. Therm Anal. Calorim. **81**, 137 (2005).
2005HUA/SIM D. Huang, S. L. Simon, and G. B. McKenna, J. Chem. Phys. **122**, 084907 (2005).
2005LV/TAN X.-C. Lv, Z.-C. Tan, Q. Shi, H.-T. Zhang, L.-X. Sun, and T. Zhang, J. Chem. Eng. Data **50**, 932 (2005).
2005MAS/NAG N. Masuda, Y. Nagano, and T. Kimura, J. Therm Anal. Calorim. **81**, 533 (2005).
2005MAT/VAN M. Matovic, J. C. van Miltenburg, J. Los, F. G. Gandolfo, and E. Floeter, J. Chem. Eng. Data **50**, 1624 (2005).
2005MOH/TAY P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**, 1 (2005).
2005PAL/ORA M. Palczewska-Tulinska and P. Orazc, J. Chem. Eng. Data **50**, 1711 (2005).
2005PAR/TOV J. M. Pardo, C. A. Tovar, J. Troncoso, E. Carbalo, and L. Romani, Thermochim. Acta **433**, 128 (2005).
2005PEL/TRO J. Peleteiro, J. Troncoso, D. Gonzales-Salgado, J. L. Valencia, M. Sonto-Caride, and L. Romani, J. Chem. Thermodyn. **37**, 935 (2005).
2005PIE/TKA1 H. Piekarski and M. Tkaczyk, Thermochim. Acta **428**, 113 (2005).
2005PIE/TKA2 H. Piekarski, M. Tkaczyk, and M. Wasiak, Therm. Sci. Eng. **82**, 711 (2005).
2005SMI/KAN N. N. Smirnova, K. V. Kandeev, and T. A. Bykova, Russ. J. Phys. Chem. **79**, 857 (2005).
2005TIA/TAN Q.-F. Tian, Z.-C. Tan, Q. Shi, F. Xu, L.-X. Sun, and T. Zhang, Thermochim. Acta **430**, 53 (2005).
2005VAL/TRO J. L. Valencia, J. Troncoso, J. Peleteiro, E. Carballo, and L. Romani, Fluid Phase Equilib. **232**, 207 (2005).
2005VAN/OON J. C. van Miltenburg and H. A. J. Oonk, J. Chem. Eng. Data **50**, 1348 (2005).
2005VAR/DRU R. M. Varushchenko, A. I. Druzhinina, V. M. Senyavin, and V. S. Sarkisova, J. Chem. Thermodyn. **37**, 141 (2005).
2005WAL/STE D. Waliszewski, I. Stepniak, H. Piekarski, and A. Lewandowski, Thermochim. Acta **433**, 149 (2005).
2005WAN/TAN1 M.-H. Wang, Z.-C. Tan, X.-H. Sun, H.-T. Zhang, B.-P. Liu, L.-X. Sun, and T. Zhang, J. Chem. Eng. Data **50**, 270 (2005).
2005WAN/TAN2 S.-X. Wang, Z.-C. Tan, Q. Shi, Y.-Y. Di, H.-T. Zhang, L.-X. Sun, and T. Zhang, J. Chem. Thermodyn. **37**, 349 (2005).
2005ZOR/CHO E. Zorebski, M. Chorazewski, and M. Tkaczyk, J. Chem. Thermodyn. **37**, 281 (2005).
2006DIE/GME A. Diedrichs and J. Gmehling, Fluid Phase Equilib. **244**, 68 (2006).
2006DRU/DOR A. I. Druzhinina, O. V. Dorofeeva, R. M. Varushchenko, and E. L. Krasnykh, J. Chem. Thermodyn. **38**, 10 (2006).
2006DZI/GOR M. Dzida and P. Goralski, J. Chem. Thermodyn. **38**, 962 (2006).
2006PAR/ZOU R. Paramo, M. Zouine, F. Sobron, and C. Casanova, J. Chem. Eng. Data **51**, 123 (2006).
2006PIE/TKA H. Piekarski and M. Tkaczyk, J. Therm Anal. Calorim. **83**, 541 (2006).
2006SHE/KAB M. P. Shevelyova, G. J. Kabo, A. V. Blokhin, A. G. Kabo, J. A. Jursha, and A. A. Rajko, J. Chem. Eng. Data **51**, 40 (2006).
2006SMI/BYK N. N. Smirnova, T. A. Bykova, K. Van Durme, and B. Van Mele, J. Chem. Thermodyn. **38**, 879 (2006).
2006SMI/KAN N. N. Smirnova, K. V. Kandeev, T. A. Bykova, and T. G. Kulagina, J. Chem. Thermodyn. **38**, 376 (2006).
2006WAN/TAN M.-H. Wang, Z.-C. Tan, Q. Shi, L.-X. Sun, and T. Zhang, J. Therm Anal. Calorim. **84**, 413 (2006).
2007FRE/HON M. L. Frenkel, X. Hong, and R. C. Wilhoit, *TRC Thermodynamic Tables. Hydrocarbons* (extant data sheets), Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, CO, 2007.
2007STR/RUZ M. Straka, K. Růžička, and V. Růžička, J. Chem. Eng. Data **52**, 1375 (2007).
2007STR/VAN M. Straka, A. C. G. van Genderen, K. Růžička, and V. Růžička, J. Chem. Eng. Data **52**, 794 (2007).