Reviews

P−ρ−*T* Data of Liquids: Summarization and Evaluation. 8. Miscellaneous Compounds

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The published experimental data for 53 compounds (eight amines, eight nitriles, four *N*-heterocyclic compounds, six nitro compounds, four amides, four other compounds containing C, H, O, and N atoms, six halogenated alcohols, five fluoroethers, and eight miscellaneous compounds) are summarized and reviewed, and the parameters of the Tait equation are given for 49 substances. This equation allows the calculation of smoothed values of either the volume ratio, $V(P)/V(P_{ref})$, and related properties (relative density, $\rho(P)/\rho(P_{ref})$, compression, $\{1 - \rho(P_{ref})/\rho(P)\}$) or, using density data at atmospheric pressure (P_{ref} = 0.1 MPa) or at saturation ($P_{ref} = P_{sat}$), the liquid densities of the substances over a temperature and pressure range. Experimental values of isothermal compressibility at atmospheric pressure compiled from the literature are also summarized and compared with values calculated from the Tait equation.

Introduction

This work is the continuation of a systematic summarization and critical evaluation of published *P*−ρ−*T* data of pure substances in the liquid state. Data for hydrocarbons C_n ($n \geq 5$) [96-cib/hne, 99-cib/tak, 99-cib/tak-1], C−H−O substances [94-cib/zik, 97-cib/hne, 97-cib/hne-1], and selected halogenated hydrocarbons [01-cib/tak] have already been reviewed and evaluated. This work concerns substances that have not been included in the previous reviews, that is, compounds of C−H−N, C−H−O−N, C−H−O−halogen, and miscellaneous substances.

Sources of Data

The original experimental data (4825 data points for 53 substances) processed were extracted from the source database which was employed for our previous reviews and is being currently updated. A list of substances is presented in Table 1 along with Chemical Abstracts Service Registry Numbers (CASRNs; provided by the authors) and formulas.

The characteristics of data that were available in the database for density and related quantities (molar and specific volumes, volume or density ratios, compression) of selected compounds are summarized in Table 2. The temperature ranges and numbers of experimental values are restricted up to the critical temperature; that is, only subcritical liquid density data were retrieved from the source database. No corrections for the different temperature scales were made; the effect is mostly less than uncertainties in density and/or temperature measurements. Besides that, very few researchers declare a particular temperature scale used (see "data type" column and footnotes *f* and *g* in Table 2). Similarly, as in our previous reviews, values (denoted by a letter F in the "data type" column of Table 2) calculated from smoothing functions presented in the papers (mostly the Tait equation), following as much as possible the information concerning the distribution of experimental points given by authors, were included for some substances if no direct experimental (D) or smoothed values (S) were available in the papers. The $\rho(T,P)$ values calculated from other properties (C) were also included in the evaluation.

Treatment of Data and Method of Data Evaluation

The procedures of treatment of the data and the critical evaluation were essentially the same as those employed in our previous papers. A brief summarization is given below.

Available data on the compressed liquid density and related quantities were fitted by a Tait equation with temperature-dependent parameters $C(T)$ and $B(T)$ written in the form

$$\rho(T,P,\vec{c},\vec{b}) = \frac{\rho(T,P_{ref}(T))}{1 - C(T,\vec{c}) \ln\left[\frac{B(T,\vec{b}) + P}{B(T,\vec{b}) + P_{ref}(T)}\right]} \quad (1)$$

where

$$C(T,\vec{c}) = \sum_{i=0}^{N_C} c_i[(T - T_0)/100]^i \qquad \vec{c} = \{c_i\} = \{c_0, ..., c_{N_C}\} \quad (2)$$

$$B(T,\vec{b}) = \sum_{i=0}^{N_B} b_i[(T - T_0)/100]^i \qquad \vec{b} = \{b_i\} = \{b_0, ..., b_{N_B}\} \quad (3)$$

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Table 1. List of Substances: Names (Alternative Names), Chemical Abstracts Service Registry Numbers, CASRN (Supplied by Authors), and Summary Formulas

name (alternative name)	CASRN	formula
C−H−N Compounds		
Amines		
1,2-ethanediamine	107-15-3	$C_2H_8N_2$
1-aminopropane (*n*-propylamine)	107-10-8	C_3H_9N
1-aminobutane (*n*-butylamine)	109-73-9	$C_4H_{11}N$
2-methyl-2-propanamine (*tert*-butylamine)	75-64-9	$C_4H_{11}N$
1-aminopentane (*n*-pentylamine)	110-58-7	$C_5H_{13}N$
aminobenzene (aniline, phenylamine)	62-53-3	C_6H_7N
2-methyl-1-aminobenzene (*o*-toluidine, 2-aminotoluene)	95-53-4	C_7H_9N
4-methyl-1-aminobenzene (*p*-toluidine, 4-aminotoluene)	106-49-0	C_7H_9N
Nitriles		
ethanenitrile (acetonitrile, methyl cyanide)	75-05-8	C_2H_3N
ethanenitrile-d_3	2206-26-0	C_2D_3N
propanenitrile (propionitrile, ethyl cyanide)	107-12-0	C_3H_5N
butanenitrile (*n*-butyronitrile, propyl cyanide)	109-74-0	C_4H_7N
2-methylpropanenitrile (*iso*-butyronitrile, 2-cyanopropane)	78-82-0	C_4H_7N
2-methylpropenenitrile (methacrylonitrile, 2-cyanopropene)	126-98-7	C_4H_5N
benzonitrile (phenyl cyanide)	100-47-0	C_7H_5N
phenylethanenitrile (α-tolunitrile, benzyl cyanide)	140-29-4	C_8H_7N
Heterocyclic C−H−N Compounds		
pyridine (azine)	110-86-1	C_5H_5N
piperidine (azacyclohexane, hexahydropyridine)	110-89-4	$C_5H_{11}N$
1-azaindene (1-benzazole, 1H-indole, benzopyrrole)	120-72-9	C_8H_7N
quinoline (benzo[*b*]pyridine)	91-22-5	C_9H_7N
C−H−O−N Compounds		
Nitro Compounds		
nitromethane	75-52-5	CH_3NO_2
nitroethane	79-24-3	$C_2H_5NO_2$
1-nitropropane	108-03-2	$C_3H_7NO_2$
2-nitropropane	79-46-9	$C_3H_7NO_2$
2-methyl-2-nitropropane	594-70-7	$C_4H_9NO_2$
nitrobenzene	98-95-3	$C_6H_5NO_2$
Amides		
formamide	75-12-7	CH_3NO
N-methylformamide	123-39-7	C_2H_5NO
N,*N*-dimethylformamide	68-12-2	C_3H_7NO
N,*N*-dimethylacetamide	127-19-5	C_4H_9NO
Other C−H−O−N Compounds		
triethanolamine	102-71-6	$C_6H_{15}NO_3$
1-methoxy-2-nitrobenzene (*o*-nitroanisole)	91-23-6	$C_7H_7NO_3$
1-methylpyrrolidin-2-one (*N*-methyl-2-pyrrolidone)	872-50-4	C_5H_9NO
3-cyanopropanal (4-oxabutanenitrile)	3515-93-3	C_4H_5NO
C−H−O Halogen Compounds		
Halogenated Alcohols		
2-fluoroethanol	371-62-0	C_2H_5FO
2,2-difluoroethanol	359-13-7	$C_2H_4F_2O$
2,2,2-trifluoroethanol	75-89-8	$C_2H_3F_3O$
2,2,3,3,3-pentafluoropropanol	422-05-9	$C_3H_3F_5O$
2,2,3,3-tetrafluoropropanol	76-37-9	$C_3H_4F_4O$
2,2,2-trichloroethanol	115-20-8	$C_2H_3Cl_3O$
Halogenated Ethers		
bis(difluoromethyl) ether (HFE134)	1691-17-4	$C_2H_2F_4O$
2,2,2-trifluoroethyl difluoromethyl ether (HFE245mf)	1885-48-9	$C_3H_3F_5O$
pentafluoroethyl methyl ether (HFE245mc)	22410-44-2	$C_3H_3F_5O$
1,2,2,2-tetrafluoroethyl difluoromethyl ether (HFE236me)	57041-67-5	$C_3H_2F_6O$
heptafluoropropyl methyl ether (HFE347mcc)	375-03-1	$C_4H_3F_7O$
Miscellaneous Compounds		
pentafluorobenzonitrile	773-82-0	C_7F_5N
tetramethylstannane	594-27-4	$C_4H_{12}Sn$
tetramethylsilane	75-76-3	$C_4H_{12}Si$
tetraethylsilane	631-36-7	$C_8H_{20}Si$
hexamethyldisilane	1450-14-2	$C_6H_{18}Si_2$
tetraethoxysilane	78-10-4	$C_8H_{20}O_4Si$
octamethylcyclotetrasiloxane	556-67-2	$C_8H_{24}O_4Si_4$
dimethyl sulfoxide	67-68-5	C_2H_6OS

and T_0 is a parameter with a preselected fixed value for which $C(T_0) = c_0$ and $B(T_0) = b_0$ are valid. The reference values, $\rho(T,P_{ref}(T))$ and $P_{ref}(T)$, were selected in the same way as that used previously; that is, at temperatures below the normal boiling temperature the densities at atmospheric pressure ($P_{ref} = 0.101\ 325$ MPa) were used, while for higher temperatures the values along the saturation curve, that is, saturated liquid densities and saturated vapor pressures, were employed. Exceptions of this rule are discussed below. Experimental values of densities at atmospheric pressure or at saturation for the same sample reported along with compressed liquid density data were preferably used for the reference density, $\rho(T,P_{ref})$, and thus, the values of relative density, $\rho(T,P)/\rho(T,P_{ref} = 0.1$ MPa or $P_{sat})$, reported by the researchers were correlated by eq 1. In some cases of isothermal data, the reference density, $\rho(T,P_{ref})$, was obtained for each isotherm by an extrapolation of experimental compressed liquid density data to the reference pressure, P_{ref} (0.101 325 MPa below or P_{sat} above the normal boiling temperature), using the Tait equation. If the reference values were not available in the original source and the extrapolation was not feasible (e.g., for isobaric or isochoric data), then densities obtained from the equations summarized in Appendix 1 (Table 6) were employed in the correlations. In the cases where the compressed-liquid data were presented in the original source in the form of one of the relative properties (relative density, $\rho(T,P)/\rho(T,P_{ref})$; volume ratio, $V(T,P)/V(T,P_{ref}) = \rho(T,P_{ref})/\rho(T,P)$; compression, $\{V(T,P_{ref}) - V(T,P)\}/V(T,P_{ref}) = 1 - \rho(T,P_{ref})/\rho(T,P)$), such data were correlated by eq 1 without any knowledge of reference densities; that is, the relative densities $\rho(T,P)/\rho(T,P_{ref})$ were correlated.

Saturated vapor pressures were calculated from the smoothing functions either taken from the literature (for references, see Table 3) or obtained by fitting to selected data (see Appendix 2 and Table 7).

Adjustable parameters $\vec{c}$ and $\vec{b}$ of function 1 were obtained by minimizing the objective function

$$\phi(\vec{c},\vec{b}) = \sum_{j=1}^{N_p} w_j[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]^2 \qquad (4)$$

where $\rho_j = \rho(T_j,P_j)$ is the jth experimental data point, $\rho(T_j,P_j,\vec{c},\vec{b})$ is the value calculated from function 1 with parameters $\vec{c}$ and $\vec{b}$ for the values T_j and P_j, and N_p is the number of experimental values of density used in the correlation. Adjustable parameters were calculated by the Marquardt algorithm in double precision to minimize the influence of rounding errors. Statistical weights, w_j, in eq 4, were defined as

$$w_j = \mu_j/(\delta\rho_j)^2 \qquad (5)$$

where $\delta\rho_j$ is the experimental uncertainty taken from the source database and either given by the authors (preferably) or estimated by a compiler for the jth density value in a correlated data set. The uncertainties $\delta\rho_j$ included not only random but also systematic error estimates (if available) and corresponded to the experimental accuracy rather than the precision of measurements. The statistical weight of each density value was adjusted by varying the parameter μ_j ($\mu_j = 0$ for rejected values), taking into account additional available information (sample purity, experimental method used, uncertainties in temperature and pressure measurements). In some cases comparisons of isothermal compressibilities calculated from the fit of a particular data set with independent values (see below and

Table 2. Characteristics of Data Sets: Overall Number of Data Points, N_p, Temperature and Pressure Ranges within the Liquid State, T_{min}, T_{max}, P_{min}, and P_{max}, Experimental Method Used, Types of Data, and Purities of Measured Samples

ref	N_p	T_{min} K	T_{max} K	P_{min} MPa	P_{max} MPa	meth[a]	data type[b]	sample purity[c] %
1,2-Ethanediamine								
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
1-Aminopropane								
95-pap/pan	9	298.15	298.15	2.0	33.9	mo	D	99.0m[e]
1-Aminobutane								
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
2-Methyl-2-aminopropane								
95-kip/woo	54	278.15	313.14	2.5	157.8	vb	D[f]	>99.5[d]
1-Aminopentane								
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
Aminobenzene								
39-gib/loe	8	298.15	358.15	50.0	100.0	va	F	
39-gib/loe-1	16	298.15	358.15	25.0	100.0	va	F	
80-tak	3	298.15	298.15	55.3	151.8	ul	C	>99.0v[e]
85-eas/woo	9	298.15	323.15	25.0	100.0	vb	S	
85-tak/ter	18	303.15	303.15	10.0	180.0	ul	F	>99.6v[e]
total	54	298.15	358.15	10.0	180.0			
2-Methyl-1-aminobenzene								
79-gus/far	60	296.50	524.00	5.0	50.0	bu	S	
4-Methyl-1-aminobenzene								
81-gus/naz	51	323.00	523.00	5.0	50.0	bu	D	
Ethanenitrile								
75-fra/fra	77	302.95	543.15	2.4	246.4	ia	D	99.8[d]
75-fra/fra	33	297.15	380.15	20.0	220.0	ia	S	99.8[d]
75-fra/fra	85	323.15	523.15	5.0	250.0	ia	S	99.8[d]
77-gup/han	24	273.15	363.15	2.8	22.1	vs	D	
77-sch/sch	21	303.15	393.15	3.0	450.0	nd	D	
77-sri/kay	12	283.15	313.15	50.0	200.0	vs	D	
79-lue/sch	8	298.15	298.15	15.0	70.0	vs	F	
80-lan/wue	20	283.15	313.15	10.0	300.0	vs	S	
80-lan/wue-1	142	233.45	313.25	10.0	300.0	vs	D	
82-eas/woo	5	298.15	298.15	50.0	250.0	vb	D	
85-eas/woo	10	298.15	313.15	50.0	250.0	vb	S	
85-kra/mue	88	256.83	523.20	0.6	60.2	ia	D[g]	99.98m[e]
88-eas/woo	83	278.15	323.15	2.5	280.0	vb	F	
90-lai/how	18	300.48	334.78	0.135	0.135	nd	D	99.9[e]
91-dym/awa	34	298.25	373.18	23.0	512.4	nd	S[h]	
total	660	233.45	543.15	0.1	512.4			
Ethanenitrile-d_3								
77-sch/sch	15	303.15	363.15	3.0	400.0	nd	D	99[d]
Propanenitrile								
84-sha/gus	102	190.36	543.18	5.0	50.0	bu	D	
90-uos/mat	6	298.15	298.15	25.0	150.0	va	D	
total	108	190.36	543.18	5.0	150.0			
Butanenitrile								
84-sha/gus	126	176.94	565.23	5.0	50.0	bu	D	
90-uos/mat	6	298.15	298.15	25.0	150.0	va	D	
total	132	176.94	565.23	5.0	150.0			
2-Methylpropanenitrile								
90-uos/mat	6	298.15	298.15	25.0	150.0	va	D	
2-Methylpropenenitrile								
83-gus/naz	25	293.00	373.00	5.0	40.0	bu	D	99.9[e]
Benzonitrile								
78-gus/naz	70	298.00	523.00	5.0	50.0	bu	D	
86-gus	15	290.00	470.00	10.0	30.0	bu	D	
90-uos/mat	6	298.15	298.15	25.0	150.0	va	D	
01-tak/fuj	13	298.15	298.15	1.7	28.6	ul	C	>99.99m[d]
total	104	290.00	523.00	1.7	150.0			
Phenylethanenitrile								
90-uos/mat	6	298.15	298.15	25.0	150.0	va	D	
Pyridine								
56-stu	1	303.15	303.15	101.3	101.3	va	D	
79-fur/mun	40	303.15	423.15	10.0	400.0	vb	S	
total	41	303.15	423.15	10.0	400.0			
Piperidine								
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
1-Azaindene								
95-yok/ebi	5	333.15	333.15	10.0	50.0	pi	D	99.9m[e]
Quinoline								
88-sid/tej	21	298.20	338.20	0.7	34.5	mo	D	>99m[d]
96-cha/lee	45	298.15	348.15	1.0	30.0	mo	D	98m[d]
96-cha/lee-1	18	333.15	413.15	5.0	30.0	mo	D	99.5[e]
96-ran/eat	40	353.15	353.15	10.0	400.0	bt	C	>99[d]
96-ran/eat	120	403.15	503.15	10.0	400.0	ca	C	>99[d]
total	244	298.15	503.15	0.7	400.0			
Nitromethane								
77-gup/han	24	273.15	363.15	2.8	22.1	vs	D	
90-uos/mat-1	12	298.15	323.15	25.0	150.0	va	D	
total	36	273.15	363.15	2.8	150.0			
Nitroethane								
77-gup/han	24	273.15	363.15	2.8	22.1	vs	D	
90-uos/mat-1	12	298.15	323.15	25.0	150.0	va	D	
total	36	273.15	363.15	2.8	150.0			
1-Nitropropane								
90-uos/mat-1	12	298.15	323.15	25.0	150.0	va	D	
2-Nitropropane								
90-uos/mat-1	12	298.15	323.15	25.0	150.0	va	D	
2-Methyl-2-nitropropane								
96-jen/reu	18	313.15	353.15	10.0	100.0	vs	S	99.5[e]
Nitrobenzene								
39-gib/loe	6	298.15	338.15	50.0	100.0	va	F	
39-gib/loe-1	16	298.15	358.15	25.0	100.0	va	F	
60-hil/goc	6	293.15	293.15	5.1	50.7	bu	D	
79-abd/dzh	63	298.15	523.15	27.7	498.2	pi	D	
82-tak/ter	25	293.15	313.15	5.0	100.0	ul	C	
90-uos/mat-1	3	298.15	298.15	25.0	75.0	va	D	
total	119	293.15	523.15	5.0	498.2			
Formamide								
83-eas/woo	74	288.15	323.15	2.2	279.7	vb	D	
89-mor/nak	1	298.15	298.15	101.3	101.3	va	D	
91-uos/kit	4	298.15	298.15	20.0	150.0	va	D	
total	79	288.15	323.15	2.2	279.7			
***N*-Methylformamide**								
85-eas/woo-1	37	288.15	313.15	2.5	290.0	vb	F	
91-uos/kit	4	298.15	298.15	50.0	200.0	va	D	
total	41	288.15	313.15	2.5	290.0			
***N*,*N*-Dimethylformamide**								
85-eas/woo-1	51	288.15	313.15	2.5	290.0	vb	F	
89-mor/nak	1	298.15	298.15	101.3	101.3	va	D	
91-uos/kit	4	298.15	298.15	20.0	150.0	va	D	
total	56	288.15	313.15	2.5	290.0			
***N*,*N*-Dimethylacetamide**								
91-uos/kit	4	298.15	298.15	50.0	200.0	va	D	
Triethanolamine								
33-bri	20	273.15	368.15	49.0	980.7	vb	D	
1-Methoxy-2-nitrobenzene								
60-hil/goc	6	293.15	293.15	6.1	48.6	bu	D	
1-Methylpyrrolidin-2-one								
91-uos/kit	4	298.15	298.15	50.0	200.0	va	D	
3-Cyanopropanal								
81-mus/gan	56	290.40	505.00	5.0	58.9	bu	D	
2-Fluoroethanol								
97-woo	134	278.15	338.13	2.4	385.8	vb	D[f]	95[d]
2,2-Difluoroethanol								
95-mal/woo	130	278.15	338.15	2.5	375.6	vb	D[g]	
2,2,2-Trifluoroethanol								
89-bae/klo	62	293.15	413.16	0.5	15.9	mo	D[g]	99.96w[d]
90-sve/sid	5	293.15	293.15	2.0	10.0	mo	D[g]	99.8[e]
91-mal/woo	138	278.15	338.15	2.5	281.7	vb	D	99.5m[d]
92-kab/yam-1	311	310.00	420.00	0.3	200.0	vb	D[f]	99.95w[e]
93-sau/hol	44	317.78	478.14	1.7	59.7	ia	D[g]	99.96[e]
93-sau/hol	35	263.15	363.15	2.0	10.0	mo	D[g]	99.96[e]
94-mat/yam	42	298.15	323.15	0.5	80.0	mo	F	>99[d]
94-mat/yam	26	298.15	323.15	0.5	40.0	mo	F	>99[d]
99-her/oli	9	343.15	423.15	1.5	1.5	mo	D	>99.9[d]
total	672	263.15	478.14	0.3	281.7			
2,2,3,3,3-Pentafluoropropanol								
94-mat/yam	42	298.15	323.15	0.5	80.0	mo	F	>99.9[d]
2,2,3,3-Tetrafluoropropanol								
94-mat/yam	42	298.15	323.15	0.5	80.0	mo	F	>99.9[d]
2,2,2-Trichloroethanol								
97-jen/san	146	290.15	355.15	10.0	290.0	vs	D	99.5[e]
Bis(difluoromethyl) Ether								
92-def/gil	57	273.58	367.31	1.0	5.3	mo	D	96.7m[e]
2,2,2-Trifluoroethyl Difluoromethyl Ether								
95-mal/woo-1	146	278.15	338.13	2.5	377.3	vb	D[f]	
Pentafluoroethyl Methyl Ether								
01-oht/mor	49	279.99	369.98	0.5	3.0	bu	D	99.99m[d]
01-wid/tsu	27	395.00	406.50	2.4	4.3	ia	D	99.9967m[d]
total	76	279.99	406.50	0.5	4.3			

Table 2. (Continued)

ref	N_p	T_{min} / K	T_{max} / K	P_{min} / MPa	P_{max} / MPa	meth[a]	data type[b]	sample purity[c] / %
1,2,2,2-Tetrafluoroethyl Difluoromethyl Ether								
95-mal/woo-1	155	278.15	338.13	2.5	375.2	vb	D[f]	
Heptafluoropropyl Methyl Ether								
01-oht/mor	80	279.99	369.98	0.5	3.0	bu	D	99.9m[d]
01-wid/uch	14	422.00	437.50	1.9	3.6	ia	D	99.4m[d]
total	94	279.99	437.50	0.5	3.6			
Pentafluorobenzonitrile								
90-pol/wei	62	283.20	363.20	5.0	200.0	vb	F	97.0[d]
Tetramethylstannane								
90-pol/wei	72	267.40	366.90	5.0	200.0	vb	F	99.0[d]
Tetramethylsilane								
75-par/jon	42	298.00	373.00	4.5	450.0	vb	D	
89-bao/cac	235	198.16	298.15	0.2	101.7	rl	D	>99.5m[e]
90-yok/tak	70	283.15	333.15	10.0	100.0	vs	D	>99m[d]
total	347	198.16	373.00	0.2	450.0			
Tetraethylsilane								
90-yok/tak	70	283.15	333.15	10.0	100.0	vs	D	>99.8m[d]
Hexamethyldisilane								
82-bri/wue	7	303.20	323.20	10.0	40.0	nd	S	>99.9[e]
Tetraethoxysilane								
90-yok/tak	70	283.15	333.15	10.0	100.0	vs	D	>99.8m[d]
Octamethylcyclotetrasiloxane								
76-ben/win	313	313.14	413.17	0.7	213.3	vb	D[h]	99.95[d]
84-eas/woo	10	323.15	323.15	5.0	80.0	vb	S	>98[d]
96-wap/tar	36	308.20	426.60	10.0	180.0	vs	D	>99[d]
total	359	308.20	426.60	0.7	213.3			
Dimethyl Sulfoxide								
80-fuc/ghe	67	293.60	323.00	5.0	150.0	vb	F	

[a] Method used for measurements: bt, calculated from compressibility; bu, buoyancy method; ca, calorimetric method; hp, high-pressure pycnometer; ia, isochoric apparatus; mo, mechanical oscillator method; nd, not described or stated in the reference; pi, piezometer of unspecified type; rl, expansion principle; ul, densities evaluated from speeds of sound; va, Aime method; vb, variable-volume cell with bellows; vs, variable-volume cell with solid piston. For the classification and description of the methods, see ref [85-tek/cib]. [b] D, direct experimental data; S, smoothed data presented in the reference; C, data calculated from other properties; F, values calculated from the smoothing equation reported by the researchers. [c] No letter, unspecified percent; m, mole percent; v, volume percent; w, mass percent. [d] Purity of source material is given only. [e] Final purity of the sample. [f] ITS-90 declared by the researchers. [g] IPTS-68 declared by the researchers. [h] Values from unpublished supplementary document.

Table 5) were made to facilitate the adjustment. The calculations of the parameters $\vec{c}$ and $\vec{b}$ were repeated until the final fit was obtained where the deviations between retained experimental and smoothed values were roughly equal to the modified experimental uncertainties, $\delta\rho_j/\mu_j^{1/2}$, that is, where the weighted standard deviation of the fit was close to unity.

Results

No results of the fits by eq 1 are presented for data reported by Hamann and Smith [71-ham/smi] where values of compression at $T = 303.15$ K and $P = 101.3$ MPa (one value per substance) are presented for 1,2-ethanediamine (0.0399), 1-aminobutane (0.0711), 1-aminopentane (0.0652), and piperidine (0.0560).

Table 3 records the values of the parameters of eq 1 for 49 substances along with some statistical information of the fits defined as follows:

$$\mathrm{RMSD} = \{\sum_{j=1}^{N_p}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]^2/N_p\}^{1/2} \quad (6)$$

$$\mathrm{RMSD_r}/\% = 100\{\sum_{j=1}^{N_p}[1 - \rho(T_j,P_j,\vec{c},\vec{b})/\rho_j]^2/N_p\}^{1/2} \quad (7)$$

$$\mathrm{bias} = \sum_{j=1}^{N_p}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})]/N_p \quad (8)$$

$$\pm = \sum_{j=1}^{N_p}\mathrm{sign}[\rho_j - \rho(T_j,P_j,\vec{c},\vec{b})] \times 1 \quad (9)$$

$$s_w = [\phi/(N_p - N_C - N_B - 2)]^{1/2} \quad (10)$$

where N_p is the overall number of experimental data points retained for the correlation. The characteristics are given on an absolute density scale ($kg\cdot m^{-3}$), which is more illustrative than on a relative density scale.

Values at high temperatures of some retained data sets were rejected in those cases where large deviations from the Tait equation were observed and it was not possible to improve the fit by additional parameters b_i and c_i. Thus, the $P-T$ ranges of some fits do not cover the entire original range of retained data sets. The temperature and/or pressure ranges were sometimes enlarged by retaining less accurate and less reliable values in the ranges beyond those of more accurate data sets but only in those cases where the representation of accurate data was not affected by the enlargement and the enlargement did not result in a distortion of the $B(T)$ function. The absence of extremes and inflection points on the function $B(T)$ (eq 3) of all final fits was checked.

The temperature and pressure ranges of validity of the fits given in the table allow one to avoid extrapolation using eq 1 with the parameters from Table 3 beyond $P-T$ areas of retained data. The $P-T$ areas that either are not rectangular or cannot be easily derived from the ranges recorded in Table 4 are shown in Figure 1, which provides crude information on the distribution of the retained data points. Nonrectangular $P-T$ areas appeared mostly for substances where the $P-T$ range approached the vicinity of a solid−liquid equilibrium line.

Table 4 summarizes some statistical information derived from the fits. Only those data subsets for which the temperature and pressure ranges are displayed in the table were retained in the correlations. The statistical characteristics of these subsets refer only to the data points retained in the correlation. On the other hand, the characteristics of the rejected subsets, that is, those for which no T and P ranges are given in the table, illustrate the deviations of the rejected points from eq 1, but only for those values within the $P-T$ areas of the retained data (see Table 3 and Figure 1). If only one set of smoothed $P-\rho-T$ values available in original sources (S- or F-type data) for a particular substance was fitted by eq 1, then average deviations of the fit (RMSD, $\mathrm{RMSD_r}$) do not reflect a real accuracy of the experiment and consequently the weighted standard deviation, s_w, may be much lower than unity.

The origin of the reference density values (RD, Table 4) is denoted by the letters “o” (original values as reported by authors of data), “p” (extrapolated from compressed-liquid data along an isotherm), and “e” (calculated from a

Table 3. Parameters c_i, b_i, and T_0 of Eq 1, Temperature and Pressure Ranges,[a] T_{min}, T_{max}, P_{min}, and P_{max}, Absolute, RMSD, and Relative, $RMSD_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, Weighted Standard Deviations, s_w, Normal Boiling Point Temperatures,[b] T_{nbp}, and References to Saturated Vapor Pressure, ref(P_{sat}), for the Fits Where $T_{max} > T_{nbp}$

	1-aminopropane	2-methyl-2-propanamine	aminobenzene	2-methyl-1-aminobenzene
c_0	0.115627	0.091578	0.094363	0.084920
b_0/MPa	99.0244	66.4473	196.3979	203.4441
b_1/(MPa K^{-1})		−64.9706	−107.3578	−151.6918
b_2/(MPa K^{-2})		13.4972	22.3750	90.1546
b_3/(MPa K^{-3})				−44.2852
b_4/(MPa K^{-4})				8.3934
T_0/K	298.15	278.15	303.15	296.50
T_{min}/K	298.15	278.15	298.15	322.50
T_{max}/K	298.15	313.14	358.15	524.00
P_{min}/MPa	2.00	2.55	10.00	5.00
P_{max}/MPa	33.90	157.82	180.00	50.00
RMSD/(kg m^{-3})	0.032	0.300	0.447	0.569
$RMSD_r$/%	0.004	0.039	0.043	0.063
bias/(kg m^{-3})	0.006	0.056	0.212	0.007
N_p	9	54	54	54
±	1	14	20	0
s_w	0.316	0.897	0.525	0.629
T_{nbp}/K	320.4	317.2	457.1	473.5
ref(P_{sat})				90-cha/gad

	4-methyl-1-aminobenzene	ethanenitrile (85-kra/mue)	ethanenitrile (full range)	ethanenitrile-d_3
c_0	2.800287	0.108788	0.102941	0.102375
c_1/K^{-1}		−0.005570	−0.002586	
b_0/MPa	5007.0371	97.2726	91.0938	81.3027
b_1/(MPa K^{-1})	−8137.4627	−80.7947	−73.7189	−64.0287
b_2/(MPa K^{-2})	4156.0076	20.5123	17.9064	6.1331
b_3/(MPa K^{-3})		−1.7929	−1.4845	
T_0/K	348.00	298.15	298.15	303.15
T_{min}/K	323.00	256.83	233.45	303.15
T_{max}/K	448.00	523.20	523.20	363.15
P_{min}/MPa	5.00	0.58	0.58	3.00
P_{max}/MPa	50.00	60.24	512.40	400.00
RMSD/(kg m^{-3})	4.618	0.129	0.719	0.471
$RMSD_r$/%	0.517	0.020	0.085	0.052
bias/(kg m^{-3})	−0.245	0.016	−0.028	−0.015
N_p	33	88	273	15
±	−1	10	15	−3
s_w	5.171	0.390	1.028	0.525
T_{nbp}/K	473.6	354.8	354.8	see text
ref(P_{sat})	90-cha/gad	77-rei/pra	77-rei/pra	

	propanenitrile	butanenitrile	2-methylpropanenitrile	2-methylpropenenitrile
c_0	0.095033	0.092174	0.098890	0.179348
b_0/MPa	86.2115	93.2663	86.7481	205.6764
b_1/(MPa K^{-1})	−73.6614	−88.3915		−234.4680
b_2/(MPa K^{-2})	47.4578	63.4215		111.3710
b_3/(MPa K^{-3})	−36.1780	−38.1743		
b_4/(MPa K^{-4})	10.8181	8.9503		
T_0/K	298.15	298.15	298.15	293.00
T_{min}/K	190.36	176.94	298.15	293.00
T_{max}/K	467.55	490.46	298.15	373.00
P_{min}/MPa	5.00	5.00	25.00	5.00
P_{max}/MPa	150.00	150.00	150.00	40.00
RMSD/(kg m^{-3})	0.535	0.992	0.307	0.376
$RMSD_r$/%	0.070	0.135	0.038	0.050
bias/(kg m^{-3})	0.019	−0.133	−0.002	0.003
N_p	60	106	6	25
±	14	−24	−2	5
s_w	0.960	2.020	3.636	0.495
T_{nbp}/K	370.5	390.5	377.0	363.4
ref(P_{sat})	83-mcg	77-rei/pra		Table 7

	benzonitrile	phenylethanenitrile	pyridine	1-azaindene
c_0	0.098882	0.155223	0.094736	0.073340
b_0/MPa	158.5407	333.9107	111.5002	144.1153
b_1/(MPa K^{-1})	−41.6826		−79.2286	
b_2/(MPa K^{-2})	−33.5808		17.1238	
b_3/(MPa K^{-3})	12.4867			
T_0/K	298.15	298.15	333.15	333.15
T_{min}/K	298.15	298.15	303.15	333.15
T_{max}/K	523.00	298.15	423.15	333.15
P_{min}/MPa	1.66	25.00	10.00	10.00
P_{max}/MPa	150.00	150.00	400.00	50.00
RMSD/(kg m^{-3})	1.633	0.241	0.529	0.193
$RMSD_r$/%	0.182	0.023	0.052	0.018
bias/(kg m^{-3})	0.074	0.005	0.098	−0.022
N_p	82	6	41	5
±	6	2	11	−1
s_w	1.995	3.585	0.461	0.838
T_{nbp}/K	463.9	506.7	388.4	527.9
ref(P_{sat})	77-rei/pra		83-mcg	

Table 3. (Continued)

	quinoline	nitromethane	nitroethane	1-nitropropane
c_0	0.091903	0.094301	0.096509	0.092543
b_0/MPa	151.4359	150.6040	145.1597	114.7628
b_1/(MPa K^{-1})	−79.1693	−81.5718	−95.5536	−76.6410
b_2/(MPa K^{-2})	9.0214	−4.8608	16.9361	
b_3/(MPa K^{-3})	4.0697			
b_4/(MPa K^{-4})	−0.6722			
T_0/K	353.15	273.15	273.15	298.15
T_{min}/K	298.15	273.15	273.15	298.15
T_{max}/K	503.15	363.15	363.15	323.15
P_{min}/MPa	1.00	2.76	2.76	25.00
P_{max}/MPa	400.00	150.00	150.00	150.00
RMSD/(kg m^{-3})	0.310	0.420	0.516	0.148
RMSD$_r$/%	0.030	0.036	0.048	0.014
bias/(kg m^{-3})	−0.045	−0.026	−0.234	0.005
N_p	143	27	36	12
±	1	−3	−16	4
s_w	1.586	1.031	1.124	1.175
T_{nbp}/K	510.3	374.3	387.2	403.3
ref(P_{sat})				

	2-nitropropane	2-methyl-2-nitropropane	nitrobenzene	formamide
c_0	0.089243	0.103218	0.093194	0.105327
b_0/MPa	100.4232	81.2663	185.0866	261.2778
b_1/(MPa K^{-1})	−67.2976	−44.4470	−96.1483	−70.3877
b_2/(MPa K^{-2})			15.6305	−70.5930
T_0/K	298.15	353.15	298.15	298.15
T_{min}/K	298.15	313.15	293.15	288.15
T_{max}/K	323.15	353.15	358.15	323.15
P_{min}/MPa	25.00	10.00	5.00	2.24
P_{max}/MPa	150.00	100.00	100.00	279.70
RMSD/(kg m^{-3})	0.112	0.501	0.065	0.213
RMSD$_r$/%	0.011	0.053	0.005	0.018
bias/(kg m^{-3})	−0.006	−0.054	0.014	0.035
N_p	12	18	50	79
±	−2	0	10	13
s_w	1.035	0.530	0.467	1.344
T_{nbp}/K	393.4	399.	483.8	483.7
ref(P_{sat})				

	N-methylformamide	*N*,*N*-dimethylformamide	*N*,*N*-dimethylacetamide	triethanolamine
c_0	0.093732	0.098235	0.092077	0.101423
c_1/K^{-1}	−0.099332			
b_0/MPa	157.6483	153.3433	142.7679	241.0284
b_1/(MPa K^{-1})	−270.2862	−81.3865		−46.4026
b_2/(MPa K^{-2})	−47.9256	−181.2935		
T_0/K	298.15	298.15	298.15	368.15
T_{min}/K	288.15	288.15	298.15	273.15
T_{max}/K	313.15	313.15	298.15	368.15
P_{min}/MPa	2.50	2.50	50.00	49.03
P_{max}/MPa	290.00	290.00	200.00	980.67
RMSD/(kg m^{-3})	0.363	0.376	0.043	0.449
RMSD$_r$/%	0.035	0.037	0.004	0.037
bias/(kg m^{-3})	−0.044	−0.058	0.000	0.021
N_p	40	44	4	20
±	−6	−4	−2	2
s_w	1.755	1.595	0.397	0.682
T_{nbp}/K	456.	425.	439.3	608.5
ref(P_{sat})				

	1-methoxy-2-nitrobenzene	1-methylpyrrolidin-2-one	3-cyanopropanal	2-fluoroethanol
c_0	0.035177	0.091074	0.090605	0.097388
b_0/MPa	42.2612	173.4791	146.7205	149.4428
b_1/(MPa K^{-1})			−105.0867	−89.8646
b_2/(MPa K^{-2})			42.7596	14.6076
b_3/(MPa K^{-3})			−11.6626	
b_4/(MPa K^{-4})			1.2509	
T_0/K	293.15	298.15	290.40	298.14
T_{min}/K	293.15	298.15	290.40	278.15
T_{max}/K	293.15	298.15	505.00	338.13
P_{min}/MPa	6.08	50.00	5.00	2.45
P_{max}/MPa	48.64	200.00	58.90	385.83
RMSD/(kg m^{-3})	0.198	0.073	0.346	0.211
RMSD$_r$/%	0.016	0.007	0.037	0.018
bias/(kg m^{-3})	0.038	−0.001	−0.016	0.074
N_p	6	4	56	134
±	0	−2	10	48
s_w	0.015	0.733	0.369	0.298
T_{nbp}/K	550.	475.	see text	376.
ref(P_{sat})				

Table 3. (Continued)

	2,2-difluoroethanol	2,2,2-trifluoroethanol	2,2,3,3,3-pentafluoropropanol	2,2,3,3-tetrafluoropropanol
c_0	0.094771	0.092911	0.078879	0.083714
c_1/K^{-1}		−0.003543		
b_0/MPa	117.2871	74.8342	61.8071	106.2015
b_1/(MPa K^{-1})	−77.9611	−58.9978	−60.6430	−88.8256
b_2/(MPa K^{-2})	11.4145	18.6097		
b_3/(MPa K^{-3})		−18.7043		
b_4/(MPa K^{-4})		8.5822		
T_0/K	313.15	298.15	298.15	298.15
T_{min}/K	278.15	263.15	298.15	298.15
T_{max}/K	338.15	433.28	323.15	323.15
P_{min}/MPa	2.55	0.49	0.50	0.50
P_{max}/MPa	375.57	281.70	80.00	80.00
RMSD/(kg m^{-3})	0.337	0.651	0.205	0.281
RMSD$_r$/%	0.025	0.049	0.013	0.019
bias/(kg m^{-3})	0.126	0.128	0.015	0.016
N_p	130	502	42	42
±	48	102	2	0
s_w	0.397	0.795	0.132	0.186
T_{nbp}/K	368	347.0	353.8	382.1
ref(P_{sat})		93-sau/hol		

	2,2,2-trichloroethanol	bis(disfluoromethyl) ether	2,2,2-trifluoroethyl difluoromethyl ether	pentafluoroethyl methyl ether
c_0	0.068406	0.086880	0.090278	0.065546
b_0/MPa	54.2989	18.2725	44.8952	21.6128
b_1/(MPa K^{-1})	−75.5685	−37.0946	−57.9641	−32.5099
b_2/(MPa K^{-2})	26.7017	16.1542	24.2391	12.1047
b_3/(MPa K^{-3})				−1.3588
T_0/K	355.15	333.12	298.14	279.99
T_{min}/K	300.15	273.58	278.15	279.99
T_{max}/K	355.15	367.31	338.13	399.00
P_{min}/MPa	10.00	1.02	2.55	0.50
P_{max}/MPa	280.00	5.30	377.31	3.01
RMSD/(kg m^{-3})	1.539	0.264	1.210	0.271
RMSD$_r$/%	0.096	0.021	0.079	0.024
bias/(kg m^{-3})	−0.017	−0.003	0.364	−0.009
N_p	134	57	145	61
±	−10	7	35	−15
s_w	0.602	0.412	0.855	0.175
T_{nbp}/K	423.	279.4	302.4	279.1
ref(P_{sat})		Table 7	98-goo/def	Table 7

	1,2,2,2-tetrafluoroethyl difluoromethyl ether	heptafluoropropyl methyl ether	pentafluorobenzonitrile	tetramethylstannane
c_0	0.089100	0.070606	0.084679	0.093735
b_0/MPa	41.9705	14.7053	89.8091	75.6897
b_1/(MPa K^{-1})	−57.6394	−29.4071	−59.6992	−64.2220
b_2/(MPa K^{-2})	22.4601	7.1925	18.5218	22.3687
b_3/(MPa K^{-3})		26.8199	−4.9729	−5.1623
T_0/K	288.15	329.99	323.40	267.40
T_{min}/K	278.15	279.99	283.20	267.40
T_{max}/K	338.13	369.98	363.20	366.90
P_{min}/MPa	2.55	0.50	5.00	5.00
P_{max}/MPa	375.20	3.01	200.00	200.00
RMSD/(kg m^{-3})	1.289	0.546	0.004	0.034
RMSD$_r$/%	0.077	0.041	0.000	0.003
bias/(kg m^{-3})	0.406	0.021	0.000	0.002
N_p	155	80	62	72
±	21	−12	4	−18
s_w	0.771	0.228	0.002	0.018
T_{nbp}/K	296.5	307.7	435.	350.7
ref(P_{sat})	Table 7	Table 7		Table 7

	tetramethylsilane	tetraethylsilane	hexamethyldisilane	tetraethoxysilane
c_0	0.090448	0.085492	0.058342	0.088030
b_0/MPa	30.4405	80.4461	21.0771	75.5983
b_1/(MPa K^{-1})	−38.7468	−56.3972	−55.6331	−57.9306
b_2/(MPa K^{-2})	19.4751	10.8974		13.3229
b_3/(MPa K^{-3})	−3.8608			
T_0/K	298.15	293.15	323.20	293.15
T_{min}/K	198.16	283.15	303.20	283.15
T_{max}/K	373.00	333.15	323.20	333.15
P_{min}/MPa	0.23	10.00	10.00	10.00
P_{max}/MPa	450.00	100.00	40.00	100.00
RMSD/(kg m^{-3})	1.646	0.122	0.654	0.145
RMSD$_r$/%	0.219	0.016	0.089	0.015
bias/(kg m^{-3})	−0.735	−0.004	0.038	−0.005
N_p	261	70	7	70
±	−157	2	3	2
s_w	1.605	0.609	1.367	0.726
T_{nbp}/K	299.8	427.9	386.	441.1
ref(P_{sat})	Table 7			

Table 3. (Continued)

	octamethylcyclotetrasiloxane	dimethyl sulfoxide
c_0	0.085893	0.105679
b_0/MPa	19.2580	186.2920
b_1/(MPa K^{-1})	−24.7486	−58.7955
b_2/(MPa K^{-2})	6.9036	
T_0/K	413.17	323.00
T_{min}/K	313.14	293.60
T_{max}/K	413.17	323.00
P_{min}/MPa	0.73	5.00
P_{max}/MPa	213.29	150.00
RMSD/(kg m^{-3})	0.320	0.438
RMSD$_r$/%	0.034	0.039
bias/(kg m^{-3})	0.023	−0.054
N_p	273	67
±	25	−5
s_w	0.562	0.398
T_{nbp}/K	448.	463.4
ref(P_{sat})		

[a] The low limit of the pressure range is 0.1 MPa or a saturation pressure (whichever is higher) for all fits. [b] Normal boiling temperature corresponds to a respective saturation pressure line or was taken from either the database [93-cda] or currently available databanks (Beilstein).

function given in Appendix 1). In some cases, the compressed-liquid data were presented in the original source in the form of a relative property (relative density, volume ratio, compression). In those cases, the reference data are also denoted as "o" in Table 4 despite the fact that the original reference density values were not known.

A comparison of isothermal compressibilities, $\beta_T = -(1/V)(\partial V/\partial P)_T = (1/\rho)(\partial\rho/\partial P)_T$, calculated from the fits for P = 0.1 MPa with available values published in the literature is presented in Table 5, which provides a rough check of the consistency of the fits with independent data. The literature values of isothermal compressibility used for the comparison in Table 5 are the values obtained either by direct measurements (not evaluated from the $P-\rho-T$ data included in the present evaluation) or from speed-of-sound measurements or adiabatic compressibility values and were either taken directly from the papers or calculated from the equation

$$\beta_T = \frac{1}{\rho}\left[\frac{1}{u^2} + \frac{TM\alpha_P^2}{c_P}\right] = \beta_S + \frac{TM\alpha_P^2}{\rho c_P} \qquad (11)$$

where M, u, α_P, β_S, and c_P are the molar mass, speed of sound, isobaric thermal expansivity ($\alpha_P = (1/V)(\partial V/\partial T)_P = -(1/\rho)(\partial\rho/\partial T)_P$), adiabatic (isoentropic) compressibility ($\beta_S = -(1/V)(\partial V/\partial P)_S = 1/(\rho u^2)$), and molar isobaric heat capacity, respectively. The values of the input quantities in eq 11 were taken from the different sources cited in Table 5. Contrary to our previous reviews, the recommended values of isobaric heat capacity [96-zab/ruz, 01-zab/ruz] for some substances are based on experimental data taken from a limited number of sources, and therefore their reliability might be rather questionable. The influence of heat capacity data on isothermal compressibility is, however, moderate, similar to the case of density values (which are usually known with an uncertainty lower than 0.1%). The uncertainty in the thermal expansivity, α_P, may have a larger effect, and therefore the values from different sources were employed where possible (see Table 5). The relative difference between isothermal and isoentropic compressibilities, $(\beta_T - \beta_S)/\beta_T$, that is, a portion of the term $TM\alpha_P^2/(\rho c_P)$ in the value of isothermal compressibility, is in the range from about 16% (formamide, 2,2,2-trifluoroethanol, both fluorinated propanols) to 30% (ethanenitrile, 2,2,2,-trichloroethanol) at temperatures close to 298 K. In a few cases, the heat capacity data of particular substances are discussed below.

No comparison is presented for 1,2-ethanediamine, 1-aminopropane, 1-aminobutane, and piperidine (either no fits were performed or an extrapolation from the fit was impossible, as for 1-aminopropane); the available isothermal compressibility values found in the literature are, however, retained in Table 5.

C−H−N Compounds. Amines. The fit of isothermal data [95-pap/pan] for 1-aminopropane gives β_T(T = 298.15 K, P = 0.1 MPa) = 1.166 GPa^{-1}. This value is lower than that calculated from speed-of-sound data [78-pat] at 293.15 K, while an opposite dependence should be expected. The isothermal compressibility of 1-aminobutane increases by about 5.6% on the 5 K increase (Table 5). Assuming the same increase for 1-aminopropane, the value β_T(T = 298.15 K, P = 0.1 MPa) = 1.27 GPa^{-1} can be derived, which is about 8% higher than that calculated from the fit. The speed-of-sound data [78-pat] seem to be correct, since, for 1,2-ethanediamine, 1-aminobutane, and 2-methyl-2-aminopropane, they are in accordance with those of other sources (Table 5).

The fit of the data for 2-methyl-2-propanamine taken from one source [95-kip/woo] gives very good agreement in isothermal compressibility (1.3% in an average, see Table 5) at T = 293.15 K, that is, at the temperature approximately in the middle of the temperature interval of the $P-\rho-T$ data.

The data available in the database for aminobenzene are in very good mutual accordance (see Table 4). Deviations in isothermal compressibility at 0.1 MPa are mostly below 1% (Table 5), even in the temperature ranges beyond the temperature interval of the fit (25 K downward, 5 K upward, see Table 5).

Data for toluidines were measured in the same laboratory. The results for 2-methyl-1-aminobenzene are better (lower RMSD, Table 3, and deviations in isothermal compressibility, Table 5) than those for 4-methyl-1-aminobenzene. Densities at atmospheric pressure reported for 2-methyl-1-aminobenzene between 296.5 and 473.6 K [79-gus/far] are by 2.9 kg·m^{-3} (RMSD) lower than those from [90-cha/gad]; the deviations for 4-methyl-1-aminobenzene [81-gus/naz] in the interval from 323 to 448 K are much greater (RMSD between [81-gus/naz] and [90-cha/gad] = 97.2 kg·m^{-3}; at T = 448 K the deviation is −155 kg·m^{-3}) and difficult to explain. Also densities extrapolated from compressed-liquid density data [81-gus/naz] to saturation pressure for temperatures higher than 473 K diverge from

Table 4. Statistical Characteristics of Individual Data Sets for the Fits in Table 3: Temperature and Pressure Ranges Taken into the Correlations, T_{min}, T_{max}, P_{min}, and P_{max}, Absolute, RMSD, and Relative, $RMSD_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, and Origin of the Reference Density Values Used in the Correlations, RD

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	$RMSD_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
				1-Aminopropane						
95-pap/pan	298.15	298.15	2.0	33.9	0.032	0.004	0.006	9	1	o
				2-Methyl-2-propanamine						
95-kip/woo	278.15	313.14	2.5	157.8	0.300	0.039	0.056	54	14	o
				Aminobenzene						
39-gib/loe	298.15	358.15	50.0	100.0	0.042	0.004	0.015	8	2	o
39-gib/loe-1	298.15	358.15	25.0	100.0	0.036	0.004	−0.016	16	−6	o
80-tak	298.15	298.15	55.3	151.8	0.031	0.003	0.028	3	3	o
85-eas/woo	298.15	323.15	25.0	100.0	0.210	0.020	0.093	9	3	o
85-tak/ter	303.15	303.15	10.0	180.0	0.759	0.073	0.593	18	18	o
				2-Methyl-1-aminobenzene						
79-gus/far	322.50	524.00	5.0	50.0	0.569	0.063	0.007	54	0	op
				4-Methyl-1-aminobenzene						
81-gus/naz	323.00	448.00	5.0	50.0	4.618	0.517	−0.245	33	−1	o
				Ethanenitrile (Fit of 85-kra/mue Data)						
75-fra/fra					7.128	1.388	−2.950	15	1	e
75-fra/fra					7.032	0.884	6.260	9	9	o
75-fra/fra					9.138	1.578	−1.092	45	3	p
77-gup/han					0.578	0.078	−0.067	24	6	p
77-sch/sch					0.630	0.094	0.449	4	2	p
77-sri/kay					1.745	0.216	−1.631	3	−3	o
79-lue/sch					0.995	0.123	−0.936	7	−7	o
80-lan/wue					0.376	0.046	−0.184	6	−2	p
80-lan/wue-1					0.655	0.079	0.190	30	12	o
82-eas/woo					0.212	0.026	−0.212	1	−1	o
85-eas/woo					0.099	0.013	0.068	2	0	o
85-kra/mue	256.83	523.20	0.6	60.2	0.129	0.020	0.016	88	10	e
88-eas/woo					0.242	0.030	−0.056	35	9	o
90-lai/how					6.682	0.871	6.451	18	18	e
91-dym/awa					1.571	0.205	−1.445	7	−7	o
				Ethanenitrile (Full Range Fit)						
75-fra/fra					14.537	1.780	8.909	66	46	e
75-fra/fra					9.239	1.092	8.572	33	33	o
75-fra/fra					11.453	1.648	2.478	85	11	p
77-gup/han	273.15	318.15	2.8	22.1	0.300	0.038	0.262	16	14	p
77-sch/sch					10.112	1.169	8.180	21	19	p
77-sri/kay					3.157	0.368	−2.825	12	−12	o
79-lue/sch					1.105	0.136	−1.037	8	−8	o
80-lan/wue	283.15	313.15	10.0	300.0	0.452	0.052	−0.299	17	−11	p
80-lan/wue-1	233.45	313.25	10.0	300.0	0.591	0.069	0.163	114	20	o
82-eas/woo	298.15	298.15	50.0	250.0	0.467	0.052	−0.237	5	−3	o
85-eas/woo	298.15	313.15	50.0	250.0	1.156	0.132	0.963	10	10	o
85-kra/mue	256.83	523.20	0.6	60.2	0.148	0.024	0.001	88	4	e
88-eas/woo					12.798	1.467	−7.980	83	−55	o
90-lai/how					6.682	0.871	6.450	18	18	e
91-dym/awa	298.25	373.18	75.5	512.4	1.867	0.221	−1.475	23	−19	o
				Ethanenitrile-d_3						
77-sch/sch	303.15	363.15	3.0	400.0	0.471	0.052	−0.015	15	−3	p
				Propanenitrile						
84-sha/gus	190.36	467.55	5.0	50.0	0.553	0.072	0.017	54	12	op
90-uos/mat	298.15	298.15	25.0	150.0	0.319	0.038	0.033	6	2	o
				Butanenitrile						
84-sha/gus	176.94	490.46	5.0	50.0	1.010	0.137	−0.140	100	−22	op
90-uos/mat	298.15	298.15	25.0	150.0	0.608	0.073	−0.009	6	−2	o
				2-Methylpropanenitrile						
90-uos/mat	298.15	298.15	25.0	150.0	0.307	0.038	−0.002	6	−2	o
				2-Methylpropenenitrile						
83-gus/naz	293.00	373.00	5.0	40.0	0.376	0.050	0.003	25	5	op
				Benzonitrile						
78-gus/naz	323.00	523.00	5.0	50.0	1.858	0.208	0.068	63	−7	op
86-gus					4.325	0.495	−1.741	12	−2	op
90-uos/mat	298.15	298.15	25.0	150.0	0.379	0.036	0.050	6	0	o
01-tak/fuj	298.15	298.15	1.7	28.6	0.126	0.012	0.113	13	13	o
				Phenylethanenitrile						
90-uos/mat	298.15	298.15	25.0	150.0	0.241	0.023	0.005	6	2	o
				Pyridine						
56-stu	303.15	303.15	101.3	101.3	0.741	0.072	−0.741	1	−1	o
79-fur/mun	303.15	423.15	10.0	400.0	0.523	0.051	0.119	40	12	op

Table 4. (Continued)

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	RMSD$_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
					1-Azaindene					
95-yok/ebi	333.15	333.15	10.0	50.0	0.193	0.018	−0.022	5	−1	o
					Quinoline					
88-sid/tej					0.346	0.032	−0.253	21	−15	o
96-cha/lee	298.15	348.15	1.0	30.0	0.107	0.010	0.002	45	11	o
96-cha/lee-1	333.15	413.15	5.0	30.0	0.176	0.017	0.048	18	6	o
96-ran/eat					4.879	0.424	4.702	40	40	o
96-ran/eat	453.15	503.15	10.0	400.0	0.398	0.039	−0.093	80	−16	o
					Nitromethane					
77-gup/han	273.15	363.15	2.8	22.1	0.234	0.021	−0.050	15	−5	p
90-uos/mat-1	298.15	323.15	25.0	150.0	0.573	0.048	0.003	12	2	o
					Nitroethane					
77-gup/han	273.15	363.15	2.8	22.1	0.630	0.059	−0.351	24	−14	p
90-uos/mat-1	298.15	323.15	25.0	150.0	0.067	0.006	−0.001	12	−2	o
					1-Nitropropane					
90-uos/mat-1	298.15	323.15	25.0	150.0	0.148	0.014	0.005	12	4	o
					2-Nitropropane					
90-uos/mat-1	298.15	323.15	25.0	150.0	0.112	0.011	−0.006	12	−2	o
					2-Methyl-2-nitropropane					
96-jen/reu	313.15	353.15	10.0	100.0	0.501	0.053	−0.054	18	0	o
					Nitrobenzene					
39-gib/loe	298.15	338.15	50.0	100.0	0.050	0.004	0.040	6	6	o
39-gib/loe-1	298.15	358.15	25.0	100.0	0.039	0.003	−0.009	16	−4	o
60-hil/goc					2.799	0.229	2.663	6	6	o
79-abd/dzh					31.053	2.615	−29.115	5	−5	o
82-tak/ter	293.15	313.15	5.0	100.0	0.068	0.006	0.033	25	9	o
90-uos/mat-1	298.15	298.15	25.0	75.0	0.138	0.011	−0.073	3	−1	o
					Formamide					
83-eas/woo	288.15	323.15	2.2	279.7	0.217	0.018	0.044	74	16	o
89-mor/nak	298.15	298.15	101.3	101.3	0.124	0.011	0.124	1	1	o
91-uos/kit	298.15	298.15	20.0	150.0	0.166	0.014	−0.138	4	−4	o
					N-Methylformamide					
85-eas/woo-1	288.15	313.15	2.5	290.0	0.375	0.036	−0.055	37	−7	o
91-uos/kit	298.15	298.15	50.0	150.0	0.134	0.013	0.099	3	1	o
					N,*N*-Dimethylformamide					
85-eas/woo-1	288.15	313.15	2.5	290.0	0.392	0.038	−0.077	39	−7	o
89-mor/nak	298.15	298.15	101.3	101.3	0.326	0.033	0.326	1	1	o
91-uos/kit	298.15	298.15	20.0	150.0	0.185	0.019	0.038	4	2	o
					N,*N*-Dimethylacetamide					
91-uos/kit	298.15	298.15	50.0	200.0	0.043	0.004	0.000	4	−2	o
					Triethanolamine					
33-bri	273.15	368.15	49.0	980.7	0.449	0.037	0.021	20	2	o
					1-Methoxy-2-nitrobenzene					
60-hil/goc	293.15	293.15	6.1	48.6	0.198	0.016	0.038	6	0	o
					1-Methylpyrrolidin-2-one					
91-uos/kit	298.15	298.15	50.0	200.0	0.073	0.007	−0.001	4	−2	o
					3-Cyanopropanal					
81-mus/gan	290.40	505.00	5.0	58.9	0.346	0.037	−0.016	56	10	op
					2-Fluoroethanol					
97woo	278.15	338.13	2.4	385.8	0.211	0.018	0.074	134	48	o
					2,2-Difluoroethanol					
95-mal/woo	278.15	338.15	2.5	375.6	0.337	0.025	0.126	130	48	o
					2,2,2-Trifluoroethanol					
89-bae/klo	313.15	413.16	0.5	15.9	0.657	0.052	−0.468	53	−33	p
90-sve/sid	293.15	293.15	2.0	10.0	0.275	0.020	−0.233	5	−5	o
91-mal/woo	278.15	338.15	2.5	281.7	0.590	0.039	0.165	138	52	o
92-kab/yam-1	350.00	420.00	0.5	200.0	0.754	0.059	0.359	195	101	o
93-sau/hol	317.78	433.28	1.7	59.7	0.897	0.071	0.113	30	8	e
93-sau/hol	263.15	363.15	2.0	10.0	0.269	0.020	0.020	35	−5	op
94-mat/yam	298.15	323.15	0.5	30.0	0.284	0.020	−0.185	20	−18	o
94-mat/yam	298.15	323.15	0.5	40.0	0.307	0.022	−0.109	26	2	o
99-her/oli					3.421	0.281	−3.213	9	−9	e
					2,2,3,3,3-Pentafluoropropanol					
94-mat/yam	298.15	323.15	0.5	80.0	0.205	0.013	0.015	42	2	o
					2,2,3,3-Tetrafluoropropanol					
94-mat/yam	298.15	323.15	0.5	80.0	0.281	0.019	0.016	42	0	o
					2,2,2-Trichloroethanol					
97-jen/san	300.15	355.15	10.0	280.0	1.539	0.096	−0.017	134	−10	p
					Bis(difluoromethyl) ether					
92-def/gil	273.58	367.31	1.0	5.3	0.264	0.021	−0.003	57	7	e

Table 4. (Continued)

ref	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	RMSD/kg·m^{-3}	RMSD$_r$/%	bias/kg·m^{-3}	N_p	±	RD[a]
2,2,2-Trifluoroethyl Difluoromethyl Ether										
95-mal/woo-1	278.15	338.13	2.5	377.3	1.210	0.079	0.364	145	35	op
Pentafluoroethyl Methyl Ether										
01-oht/mor	279.99	369.98	0.5	3.0	0.291	0.024	−0.006	49	−13	o
01-wid/tsu	395.00	399.00	2.4	2.7	0.162	0.020	−0.020	12	−2	e
1,2,2,2-Tetrafluoroethyl Difluoromethyl Ether										
95-mal/woo-1	278.15	338.13	2.5	375.2	1.289	0.077	0.406	155	21	op
Heptafluoropropyl Methyl Ether										
01-oht/mor	279.99	369.98	0.5	3.0	0.546	0.041	0.021	80	−12	o
01-wid/uch								0	0	
Pentafluorobenzonitrile										
90-pol/wei	283.20	363.20	5.0	200.0	0.004	0.000	0.000	62	4	o
Tetramethylstannane										
90-pol/wei	267.40	366.90	5.0	200.0	0.034	0.003	0.002	72	−18	o
Tetramethylsilane										
75-par/jon	348.00	373.00	10.4	450.0	4.886	0.641	−3.381	21	−15	p
89-bao/cac	198.16	268.11	0.2	101.7	1.057	0.144	−0.717	170	−128	o
90-yok/tak	283.15	333.15	10.0	100.0	0.485	0.069	0.017	70	−14	p
Tetraethylsilane										
90-yok/tak	283.15	333.15	10.0	100.0	0.122	0.016	−0.004	70	2	p
Hexamethyldisilane										
82-bri/wue	303.20	323.20	10.0	40.0	0.654	0.089	0.038	7	3	o
Tetraethoxysilane										
90-yok/tak	283.15	333.15	10.0	100.0	0.145	0.015	−0.005	70	2	p
Octamethylcyclotetrasiloxane										
76-ben/win	313.14	413.17	0.7	213.3	0.320	0.034	0.023	273	25	o
84-eas/woo					3.678	0.376	−3.432	10	−10	o
96-wap/tar					2.776	0.286	1.738	22	12	p
Dimethyl Sulfoxide										
80-fuc/ghe	293.60	323.00	5.0	150.0	0.438	0.039	−0.054	67	−5	o

[a] o, original reference density values as reported by authors were used or relative property (relative density, volume ratio, compression) was correlated by eq 1; p, reference values were obtained by the extrapolation of isothermal compressed-liquid data to reference pressure using eq 1; e, reference density values were calculated from functions given in Appendix 1.

the recommended values [90-cha/gad]. Unusual values of the parameters of the Tait equation (Table 3) also support the conclusion that the data for 4-methyl-1-aminobenzene [81-gus/naz] are highly suspicious.

Nitriles. Two fits are presented for ethanenitrile. The first one represents the data of Kratzke and Mueller [85-kra/mue], which give lower deviations of the fit (RMSD, Table 3) and better agreement in isothermal compressibility (Table 5) in the low temperature region. The second fit ("full range fit") extends both the temperature and pressure ranges, but the representation of data [85-kra/mue] is not significantly affected (see Table 4). A printing error was corrected in the data set [85-eas/woo] (volume ratio at 313.15 K and 250 MPa should be 0.8546, not 0.7546).

No information on normal boiling point temperature nor saturated vapor pressure was available for ethanenitrile-d_3. Therefore, the reference pressure $P_{ref} = 0.101\ 325$ MPa was assumed for the entire temperature range of data [77-sch/sch], which might be close to reality, since the normal boiling point temperature can be expected to be higher than that of ethanenitrile (354.8 K). It should be pointed out that the data [77-sch/sch] for ethanenitrile were rejected because of large positive deviations from other data at high pressures (see Table 4).

The fit of the two data sets available for propanenitrile gives good agreement for isothermal compressibilities at ambient temperatures (Table 5); the average deviation (positive) is 0.4%. A separate fit of isothermal data [90-uos/mat] resulted in $c_0 = 0.095\ 419$, $b_0 = 86.6719$ MPa, $T_{min} = T_{max} = 298.15$ K, $P_{min} = 25.00$ MPa, $P_{max} = 150.00$ MPa, RMSD = 0.316 kg·m^{-3}, and RMSD$_r$ = 0.037%. The isothermal compressibility calculated from this fit [β_T(T = 298.15 K, P = 0.1 MPa) = 1.100 GPa^{-1}] is by 0.1% higher than the value obtained by the linear interpolation of literature values (Table 5).

Data of the same origin as for propanenitrile were available for butanenitrile; the mutual agreement is, however, rather worse (see RMSD in Table 4). The calculated isothermal compressibilities at 293.15 and 303.15 K are significantly lower than the literature data (average deviation 5%, Table 5). Similarly, a separate fit of the isothermal data [90-uos/mat] was performed: $c_0 = 0.091\ 501$, $b_0 = 92.3304$ MPa, $T_{min} = T_{max} = 298.15$ K, $P_{min} = 25.00$ MPa, $P_{max} = 150.00$ MPa, RMSD = 0.614 kg·m^{-3}, RMSD$_r$ = 0.073%. The isothermal compressibility calculated from this fit β_T(T = 298.15 K, P = 0.1 MPa) = 0.990 GPa^{-1} is by 4.7% lower than the value obtained by the linear interpolation of data from Table 5. The recommended values of heat capacities [96-zab/ruz] are based on the data of Mirzaliev et al. [87-mir/sha]. The value reported in 1902 by Longinine (*Ann. Chim. Phys.* **1902**, *27*, 105) [02-zab] as the mean heat capacity in the range from 294.3 to 386.5 K (158.2 J·mol^{-1}·K^{-1}) is by 12% higher than the mean value [87-mir/sha] in the range from 293 to 373 K (140.6 J·mol^{-1}·K^{-1}). If the values of Mirzaliev et al. [87-mir/sha] increased by 12% are used in eq 11, then the average deviation of isothermal compressibilities calculated from the fit in Table 3 from those calculated from eq 11 would decrease to 2.5% (remaining, however, negative).

Table 5. Selected Values of Isothermal Compressibility, $\beta_T = (1/\rho)(\partial\rho/\partial P)_T$, at $P = 0.1$ MPa from the Literature and Comparison with Values Calculated from the Fits in Table 3 (Eq 1)

	β_T/GPa^{-1}				β_T/GPa^{-1}			
T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref(s)	T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref(s)
			1,2-Ethanediamine					4-Methyl-1-aminobenzene	
293.00		0.493		84-kar/bus[c]	333.15	0.444 ± 0.070	0.658	−32.5	49-bac,[d]90-cha/gad,[f,g] 96-zab/ruz[h]
293.15		0.494		78-pat,[d,e] 48-vog,[f,g] 96-zab/ruz[h]			0.664	−33.1	49-bac,[e]90-cha/gad,[f,g] 96-zab/ruz[h]
298.00		0.508		84-kar/bus[c]				Ethanenitrile (Fit of Data 85-kra/mue)	
298.15		0.490		93-rod[c]	273.15	0.927 ± 0.004	0.909	2.0	49-lag/mcm,[d]i, 96-zab/ruz[h]
303.15		0.531		81-rao/kri,[d,e] 48-vog,[f,g] 96-zab/ruz[h]			0.916	1.2	84-nie,[d]i, 96-zab/ruz[h]
					283.15	0.997 ± 0.004	0.987	1.0	49-lag/mcm,[d]i, 96-zab/ruz[h]
313.00		0.572		84-kar/bus[c]			0.994	0.3	84-nie,[d]i, 96-zab/ruz[h]
333.00		0.651		84-kar/bus[c]	293.15	1.075 ± 0.004	1.068	0.7	78-pat,[d,e] i, 96-zab/ruz[h]
			1-Aminopropane				1.072	0.3	49-lag/mcm,[d]i, 96-zab/ruz[h]
293.15		1.202		78-pat,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.074	0.1	44-sch,[d,e] i, 96-zab/ruz[h]
		1.205		78-pat,[e]90-cha/gad,[f,g] 96-zab/ruz[h]			1.079	−0.4	84-nie,[d]i, 96-zab/ruz[h]
			1-Aminobutane		298.00	1.116 ± 0.005	1.122	−0.5	95-gil/sin,[d,e] i, 96-zab/ruz[h]
293.15		1.049		78-pat,[d]93-das/fre,[f,g] 96-zab/ruz[h]	298.15	1.117 ± 0.005	1.112	0.5	47-wil,[d]i, 96-zab/ruz[h]
		1.052		78-pat,[e]93-das/fre,[f,g] 96-zab/ruz[h]			1.114	0.3	65-for/moo,[d,e] 96-ara/jad,[d,e] i, 96-zab/ruz[h]
		1.056		67-mar,[e]93-das/fre,[f,g] 96-zab/ruz[h]					
298.15		1.109		97-dom/lop,[d]93-das/fre,[f,g] 96-zab/ruz[h]			1.115	0.2	98-cha/kum,[d]i, 96-zab/ruz[h]
							1.116	0.1	93-nak/chu,[c]93-nak/chu-1[c]
		1.117		97-dom/lop,[e]93-das/fre,[f,g] 96-zab/ruz[h]			1.117	0.0	92-miy/tam[c]
							1.120	−0.3	95-ami/gop,[d,e] i, 96-zab/ruz[h]
			2-Methyl-2-aminopropane				1.125	−0.7	86-bot/bre[c]
293.15	1.604 ± 0.017	1.570	2.2	78-pat,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]			1.125	−0.7	84-nie,[d] 92-miy/tam,[d,e] 93-nak/chu,[d,e] 93-nak/chu-1,[d,e] 95-nak/tam,[d,e] i, 96-zab/ruz[h]
		1.598	0.4	67-mar,[e]93-das/fre,[f,g] 96-zab/ruz[h]					
		1.614	−0.6	67-mar,[d]93-das/fre,[f,g] 96-zab/ruz[h]					
			Aminobenzene				1.126	−0.8	81-ben/d′a,[d]i, 96-zab/ruz[h]
273.15	0.409[n]	0.405	1.0	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.154	−3.2	76-gra/mac[c]
							1.160	−3.7	76-gra/mac,[j]i
		0.408	0.2	14-tyr[c]	303.00	1.161 ± 0.005	1.169	−0.7	00-abr/abd,[e]i, 96-zab/ruz[h]
283.15	0.431[n]	0.429	0.5	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.170	−0.8	00-abr/abd,[d]i, 96-zab/ruz[h]
303.15	1.162 ± 0.005	1.161	0.9	95-osw/pat[c]					
		0.430	0.2	14-tyr[c]			1.167	−0.4	49-lag/mcm,[d]i, 96-zab/ruz[h]
		0.431	0.0	71-ric/rog[c]			1.168	−0.5	93-rao/rao,[d,e] i, 96-zab/ruz[h]
293.15	0.455[n]	0.448	1.6	24-bus,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.172	−0.9	81-nar/dha,[d,e] 95-osw/pat-1,[d,e] 00-osw/pat,[d,e] i, 96-zab/ruz[h]
		0.453	0.4	14-tyr[c]					
		0.454	0.2	71-ric/rog[c]					
		0.455	0.0	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.173	−0.9	92-dew/meh,[d,e] i, 96-zab/ruz[h]
		0.456	−0.2	44-sch,[d]71-des/bha-1,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.174	−1.0	84-nie,[d]i, 96-zab/ruz[h]
308.00	1.208 ± 0.005	1.221	−1.1	00-abr/abd,[e]i, 96-zab/ruz[h]					
		0.457	−0.4	52-jac[c]			1.223	−1.2	95-gil/sin,[d,e] i, 96-zab/ruz[h]
293.25	0.455[n]	0.456	−0.2	52-gab/poi,[d,e] 90-cha/gad,[f,g] 96-zab/ruz[h]			1.224	−1.3	00-abr/abd,[d]i, 96-zab/ruz[h]
308.15	1.209 ± 0.005	1.205	0.3	76-gra/mac[c]					
297.15	0.465[n]	0.460	1.1	62-red/sub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.215	−0.5	76-gra/mac,[j]i
313.00	1.258 ± 0.006	1.277	−1.5	00-abr/abd,[e]i, 96-zab/ruz[h]					
297.95	0.467[n]	0.466	0.2	53-par/bak,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.280	−1.7	00-abr/abd,[d]i, 96-zab/ruz[h]
313.15	1.260 ± 0.006	1.271	−0.9	49-lag/mcm,[d]i, 96-zab/ruz[h]					
298.15	0.467 ± 0.001	0.469	−0.4	71-des/bha[c]			1.279	−1.5	84-nie,[d]i, 96-zab/ruz[h]
		0.470	−0.6	52-gab/poi,[d,e] 80-tak,[d] 90-cha/gad,[f,g] 96-zab/ruz[h]	318.00	1.311 ± 0.006	1.332	−1.6	95-gil/sin,[d]i, 96-zab/ruz[h]
							1.334	−1.7	95-gil/sin,[e]i, 96-zab/ruz[h]
303.00	0.480 ± 0.001	0.483	−0.6	92-kan/raj,[d,e] 90-cha/gad,[f,g] 96-zab/ruz[h]	318.15	1.313 ± 0.006	1.300	1.0	76-gra/mac[c]
323.15	1.369 ± 0.006	1.387	−1.3	49-lag/mcm,[d]i, 96-zab/ruz[h]					
303.15	0.480 ± 0.001	0.477	0.6	14-tyr,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.397	−2.0	84-nie,[d]i, 96-zab/ruz[h]
		0.480	0.0	78-tak,[d]85-tak/ter,[d]90-cha/gad,[f,g] 96-zab/ruz[h]	326.15	1.405 ± 0.006	1.399	0.4	76-gra/mac,[j]i
333.15	1.494 ± 0.006	1.516	−1.5	49-lag/mcm,[d]i, 96-zab/ruz[h]					
		0.482	−0.4	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.527	−2.2	84-nie,[d]i, 96-zab/ruz[h]
								Ethanenitrile (Full Range Fit)	
308.15	0.494 ± 0.001	0.494	0.0	71-des/bha[c]	273.15	0.935 ± 0.003	0.909	2.9	49-lag/mcm,[d]i, 96-zab/ruz[h]
		0.495	−0.2	85-raj/ram,[d,e] 90-cha/gad,[f,g] 96-zab/ruz[h]			0.916	2.1	84-nie,[d]i, 96-zab/ruz[h]
283.15	1.006 ± 0.004	0.987	2.0	49-lag/mcm,[d]i, 96-zab/ruz[h]					
		0.499	−1.0	71-des/bha-1,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			0.994	1.2	84-nie,[d]i, 96-zab/ruz[h]
293.15	1.086 ± 0.004	1.068	1.7	78-pat,[d,e] i, 96-zab/ruz[h]					
313.15	0.507 ± 0.001	0.504	0.6	14-tyr[c]			1.072	1.3	49-lag/mcm,[d]i, 96-zab/ruz[h]
		0.510	−0.6	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]			1.074	1.1	44-sch,[d,e] i, 96-zab/ruz[h]
							1.079	0.6	84-nie,[d]i, 96-zab/ruz[h]
318.15	0.522 ± 0.001	0.523	−0.2	71-des/bha[c]	298.00	1.127 ± 0.004	1.122	0.4	95-gil/sin,[d,e] i, 96-zab/ruz[h]
323.15	0.536 ± 0.001	0.532	0.8	14-tyr[c]	298.15	1.129 ± 0.004	1.112	1.5	47-wil,[d]i, 96-zab/ruz[h]
		0.534	0.4	71-ric/rog[c]			1.114	1.3	65-for/moo,[d,e] 96-ara/jad,[d,e] i, 96-zab/ruz[h]
		0.541	−0.9	29-fry/hub,[d]90-cha/gad,[f,g] 96-zab/ruz[h]					
							1.115	1.3	98-cha/kum,[d]i, 96-zab/ruz[h]
							1.116	1.2	93-nak/chu,[c]93-nak/chu-1[c]
333.15	0.567 ± 0.002	0.564	0.5	14-tyr[c]			1.117	1.1	92-miy/tam[c]
343.15	0.601 ± 0.002	0.597	0.7	14-tyr[c]			1.120	0.8	95-ami/gop,[d,e] i, 96-zab/ruz[h]
353.15	0.636 ± 0.002	0.632	0.6	14-tyr[c]			1.125	0.4	86-bot/bre[c]
363.15	0.673[n]	0.670	0.4	14-tyr[c]			1.125	0.4	84-nie,[d] 92-miy/tam,[d,e] 93-nak/chu,[d,e] 93-nak/chu-1,[d,e] 95-nak/tam,[d,e] i, 96-zab/ruz[h]
			2-Methyl-1-aminobenzene						
293.15	0.407[n]	0.465	−12.5	24-bus,[d]90-cha/gad,[f,g] 96-zab/ruz[h]					
		0.470	−13.4	44-sch,[d]52-jac,[d,e] 90-cha/gad,[f,g] 96-zab/ruz[h]			1.126	0.3	81-ben/d′a,[d]i, 96-zab/ruz[h]
							1.154	−2.2	76-gra/mac[c]
333.15	0.537 ± 0.016	0.612	−12.3	49-bac,[d,e] 90-cha/gad,[f,g] 96-zab/ruz[h]			1.160	−2.7	76-gra/mac,[j]i

Table 5. (Continued)

T/K	β_T/GPa^{-1} eq 1[a]	β_T/GPa^{-1} lit.	$\delta\beta_T$/%[b]	ref(s)
		Ethanenitrile (Full Range Fit Continued)		
303.00	1.173 ± 0.004	1.169	0.3	00-abr/abd,[e] i, 96-zab/ruz[h]
		1.170	0.3	00-abr/abd,[d] i, 96-zab/ruz[h]
303.15	1.174 ± 0.004	1.161	1.1	95-osw/pat[c]
		1.167	0.6	49-lag/mcm,[d] i, 96-zab/ruz[h]
		1.168	0.5	93-rao/rao,[d,e] i, 96-zab/ruz[h]
		1.172	0.2	81-nar/dha,[d,e] 95-osw/pat-1,[d,e] 00-osw/pat,[d,e] i, 96-zab/ruz[h]
		1.173	0.1	92-dew/meh,[d,e] i, 96-zab/ruz[h]
		1.174	0.0	84-nie,[d] i, 96-zab/ruz[h]
308.00	1.221 ± 0.004	1.221	0.0	00-abr/abd,[e] i, 96-zab/ruz[h]
		1.223	−0.2	95-gil/sin,[d,e] i, 96-zab/ruz[h]
		1.224	−0.2	00-abr/abd,[d] i, 96-zab/ruz[h]
308.15	1.222 ± 0.004	1.205	1.4	76-gra/mac[c]
		1.215	0.6	76-gra/mac,[j] i
313.00	1.272 ± 0.004	1.277	−0.4	00-abr/abd,[e] i, 96-zab/ruz[h]
		1.280	−0.6	00-abr/abd,[d] i, 96-zab/ruz[h]
313.15	1.273 ± 0.004	1.271	0.2	49-lag/mcm,[d] i, 96-zab/ruz[h]
		1.279	−0.5	84-nie,[d] i, 96-zab/ruz[h]
318.00	1.326 ± 0.004	1.332	−0.5	95-gil/sin,[d] i, 96-zab/ruz[h]
		1.334	−0.6	95-gil/sin,[e] i, 96-zab/ruz[h]
318.15	1.327 ± 0.004	1.300	2.1	76-gra/mac[c]
323.15	1.385 ± 0.004	1.387	−0.1	49-lag/mcm,[d] i, 96-zab/ruz[h]
		1.397	−0.9	84-nie,[d] i, 96-zab/ruz[h]
326.15	1.421 ± 0.004	1.399	1.6	76-gra/mac,[j] i
333.15	1.511 ± 0.004	1.516	−0.3	49-lag/mcm,[d] i, 96-zab/ruz[h]
		1.527	−1.0	84-nie,[d] i, 96-zab/ruz[h]
		Propanenitrile		
293.15	1.055 ± 0.005	1.050	0.5	78-pat,[d,e] i, 96-zab/ruz[h]
		1.051	0.4	78-pat,[d,e] 84-sha/gus[f,g], 96-zab/ruz[h]
303.15	1.149 ± 0.006	1.145	0.3	95-osw/pat,[d,e] 95-osw/pat-1,[d,e] 84-sha/gus[f,g] 96-zab/ruz[h]
		1.148	0.1	95-osw/pat,[d,e] 95-osw/pat-1,[d,e] i, 96-zab/ruz[h]
		Butanenitrile		
293.15	0.941 ± 0.010	0.984	−4.4	78-pat,[d,e] i, 96-zab/ruz[h]
		1.005	−6.4	78-pat,[d,e] 84-sha/gus[f,g], 96-zab/ruz[h]
303.15	1.035 ± 0.010	1.074	−3.6	92-dew/meh,[d,e] i, 96-zab/ruz[h]
		1.091	−5.1	92-dew/meh,[d,e] 84-sha/gus[f,g], 96-zab/ruz[h]
		Benzonitrile		
283.15	0.603[n]	0.588	2.6	01-tak/fuj,[d] i, 96-zab/ruz[h]
293.15	0.616[n]	0.606	1.7	78-pat,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.622	−1.0	78-pat,[d,e] i, 96-zab/ruz[h]
298.00	0.623[n]	0.626	−0.5	95-gil/sin,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.642	−3.0	95-gil/sin,[d,e] i, 96-zab/ruz[h]
298.15	0.623 ± 0.009	0.628	−0.8	88-tak/ter,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.643	−3.1	88-tak/ter,[d] 01-tak/fuj,[d] i, 96-zab/ruz[h]
		0.649	−4.0	01-tak/fuj[c]
303.00	0.632 ± 0.009	0.639	−1.1	00-abr/abd,[e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.641	−1.4	00-abr/abd,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.655	−3.5	00-abr/abd,[e] i, 96-zab/ruz[h]
		0.657	−3.8	00-abr/abd,[d] i, 96-zab/ruz[h]
303.15	0.632 ± 0.009	0.647	−2.3	88-tak/ter,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.663	−4.7	88-tak/ter,[d] i, 96-zab/ruz[h]
308.00	0.641 ± 0.010	0.659	−2.7	00-abr/abd,[e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.661	−3.0	00-abr/abd,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.667	−3.9	95-gil/sin,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.675	−5.0	00-abr/abd,[e] i, 96-zab/ruz[h]
		0.678	−5.5	00-abr/abd,[d] i, 96-zab/ruz[h]
		0.683	−6.1	95-gil/sin,[d,e] i, 96-zab/ruz[h]
		Benzonitrile (Continued)		
308.15	0.641 ± 0.010	0.665	−3.6	85-raj/ram,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.670	−4.3	82-kar/red,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.681	−5.9	85-raj/ram,[d,e] i, 96-zab/ruz[h]
		0.686	−6.6	82-kar/red,[d,e] i, 96-zab/ruz[h]
313.00	0.652 ± 0.011	0.680	−4.1	00-abr/abd,[e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.682	−4.4	00-abr/abd,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.697	−6.5	00-abr/abd,[e] i, 96-zab/ruz[h]
		0.699	−6.7	00-abr/abd,[d] i, 96-zab/ruz[h]
313.15	0.652 ± 0.011	0.690	−5.5	01-tak/fuj,[d] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.706	−7.6	01-tak/fuj,[d] i, 96-zab/ruz[h]
318.00	0.663 ± 0.014	0.708	−6.4	95-gil/sin,[d,e] 78-gus/naz,[f,g] 86-gus,[f,g] 96-zab/ruz[h]
		0.725	−8.6	95-gil/sin,[d,e] i, 96-zab/ruz[h]
		Pyridine		
293.15	0.649[n]	0.673	−3.6	71-ric/rog[c]
		0.682	−4.8	71-des/bha-1,[d] 93-das/fre,[f,g] 96-zab/ruz[h]
298.00	0.669[n]	0.703	−4.8	95-gil/sin,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
298.15	0.670[n]	0.700	−4.3	82-gri/phi[g,j]
		0.704	−4.8	47-wil,[e] 93-das/fre,[f,g] 96-zab/ruz[h]
		0.706	−5.1	47-wil,[d] 93-das/fre,[f,g] 96-zab/ruz[h]
303.15	0.692 ± 0.006	0.720	−3.9	62-red/sub,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		0.726	−4.7	96-nat,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		0.729	−5.1	96-nat[c]
308.00	0.714 ± 0.006	0.748	−4.5	95-gil/sin,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
318.00	0.764 ± 0.006	0.797	−4.1	95-gil/sin,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		Piperidine		
293.15	-	0.778	-	78-pat,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		Quinoline		
298.55	0.467 ± 0.011	0.481	−2.9	53-par/bak,[d] 93-das/fre,[f,g] 96-zab/ruz[h]
303.15	0.477 ± 0.009	0.486	−1.9	88-dew/sha[c]
		0.492	−3.0	92-nat/tev,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		0.493	−3.2	86-nat/sin,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
313.15	0.499 ± 0.006	0.516	−3.3	86-nat/sin,[d,e] 92-nat/tev,[d,e] 93-das/fre,[f,g] 96-zab/ruz[h]
		Nitromethane		
274.10	0.629 ± 0.011	0.617	1.9	80-vit/ber,[d,e,f,g] 96-zab/ruz[h]
		0.626	0.5	80-vit/ber,[d,e] i, 96-zab/ruz[h]
278.20	0.643 ± 0.010	0.635	1.3	80-vit/ber,[d,e,f,g] 96-zab/ruz[h]
		0.644	−0.2	80-vit/ber,[d,e] i, 96-zab/ruz[h]
282.70	0.660 ± 0.009	0.654	0.9	80-vit/ber,[d,e,f,g] 96-zab/ruz[h]
		0.662	−0.3	80-vit/ber,[d] i, 96-zab/ruz[h]
		0.665	−0.8	80-vit/ber,[e] i, 96-zab/ruz[h]
283.15	0.662 ± 0.008	0.656	0.9	01-tro/tov,[d,e] i, 96-zab/ruz[h]
288.15	0.682 ± 0.007	0.678	0.6	00-cer/tov,[e] 01-tro/tov,[d,e] i, 96-zab/ruz[h]
290.00	0.689 ± 0.006	0.679	1.5	80-vit/ber,[d,e,f,g] 96-zab/ruz[h]
		0.688	0.1	80-vit/ber,[d] i, 96-zab/ruz[h]
		0.690	−0.1	80-vit/ber,[e] i, 96-zab/ruz[h]
293.15	0.703 ± 0.006	0.696	1.0	52-jac,[c,e] i, 96-zab/ruz[h]
		0.697	0.9	44-sch,[d,e] i, 96-zab/ruz[h]
		0.701	0.3	00-cer/tov[e,f,g,h]
		0.702	0.1	01-tro/tov,[d,e] i, 96-zab/ruz[h]
298.15	0.725 ± 0.006	0.718	1.0	47-wil,[d,e] i, 96-zab/ruz[h]
		0.720	0.7	01-tro/tov,[d,e,f,g] 96-zab/ruz[h]
		0.727	−0.3	01-tro/tov,[d,e] i, 96-zab/ruz[h]
		0.729	−0.5	00-cer/tov[c]
303.15	0.750 ± 0.006	0.750	0.0	92-dew/meh,[d,e] i, 96-zab/ruz[h]
		0.752	−0.3	01-tro/tov,[d,e] i, 96-zab/ruz[h]
		0.796	−5.8	88-dew/sha[c]
308.15	0.776 ± 0.006	0.779	−0.4	00-cer/tov[e,f,g,h]
		0.780	−0.5	01-tro/tov,[d,e,f,g] 96-zab/ruz[h]

Table 5. (Continued)

	β_T/GPa^{-1}					β_T/GPa^{-1}				
T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref(s)	T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref(s)
				Nitroethane					*N*-Methylformamide
283.15	0.711 ± 0.003	0.717	−0.8	00-tro/car,[d,e,f,g] 96-zab/ruz[h]	298.15	0.594 ± 0.007	0.593	0.2	77-kaw/ohn,[d,e] 94-pal/sin,[d,e]
286.15	0.725 ± 0.003	0.733	−1.1	00-tro/car,[d,e,f,g] 96-zab/ruz[h]					85-eas/woo-1,[f,g] 96-zab/ruz[h]
288.15	0.735 ± 0.002	0.745	−1.3	00-tro/car,[d,e,f,g] 96-zab/ruz[h]			0.595	−0.2	86-bot/bre[c,k]
291.15	0.750 ± 0.002	0.762	−1.6	00-tro/car,[d,e,f,g] 96-zab/ruz[h]			0.598	−0.7	77-kaw/ohn,[d,e] 94-pal/sin,[d,e]
293.15	0.761 ± 0.002	0.774	−1.7	00-tro/car,[d,e,f,g] 96-zab/ruz[h]					91-pac,[f,g] 96-zab/ruz[h]
296.15	0.777 ± 0.002	0.792	−1.9	00-tro/car,[d,e,f,g] 96-zab/ruz[h]			0.608	−2.3	86-bot/bre[c,k]
298.15	0.788 ± 0.002	0.805	−2.1	00-tro/car,[d,e,f,g] 96-zab/ruz[h]	308.15	0.643 ± 0.007	0.622	3.4	77-kaw/ohn,[d,e] 85-eas/woo-1,[f,g] 96-zab/ruz[h]
301.15	0.805 ± 0.002	0.824	−2.3	00-tro/car,[d,e,f,g] 96-zab/ruz[h]			0.627	2.6	77-kaw/ohn,[d,e] 91-pac,[f,g] 96-zab/ruz[h]
303.15	0.817 ± 0.002	0.837	−2.4	00-tro/car,[d,e,f,g] 96-zab/ruz[h]					*N*,*N*-Dimethylformamide
		0.841	−2.9	92-dew/meh,[d,e] 00-tro/car,[f,g]	293.15	0.625 ± 0.005	0.605	3.3	87-abd/mun[c]
				96-zab/ruz[h]			0.613	2.0	76-zel/dya,[d,e] i, 96-zab/ruz[h]
		0.849	−3.8	88-dew/sha[c]			0.617	1.3	76-zel/dya,[d,e] 85-eas/woo-1,[f,g]
306.15	0.835 ± 0.002	0.856	−2.5	00-tro/car,[d,e,f,g] 96-zab/ruz[h]					96-zab/ruz[h]
308.15	0.847 ± 0.002	0.869	−2.5	00-tro/car,[d,e,f,g] 96-zab/ruz[h]	298.15	0.640 ± 0.004	0.628	1.9	98-ami/pat,[d,e] i, 96-zab/ruz[h]
				1-Nitropropane			0.632	1.3	98-ami/pat,[d,e] 85-eas/woo-1,[f,g]
303.15	0.833 ± 0.003	0.839	−0.7	88-dew/sha[c]					96-zab/ruz[h]
				2-Nitropropane			0.642	−0.3	75-dac/bir,[c]98-cha/kum,[d,e] i,
303.15	0.919 ± 0.004	0.964	−4.7	88-dew/sha[c]					96-zab/ruz[h]
				Nitrobenzene			0.644	−0.6	97-ara/jad,[d,e] i, 96-zab/ruz[h]
273.15	0.443[n]	0.441	0.5	14-tyr[c]			0.646	−0.9	98-cha/kum,[d,e] 85-eas/woo-1,[f,g]
280.65	0.460[n]	0.462	−0.4	46-pel/gal,[d]i, 96-zab/ruz[h]					96-zab/ruz[h]
283.15	0.466[n]	0.467	−0.2	14-tyr[c]			0.647	−1.1	77-kaw/ohn,[d,e] i, 96-zab/ruz[h]
293.15	0.490 ± 0.001	0.478	2.5	24-bus,[d,e] i, 96-zab/ruz[h]			0.648	−1.2	94-pal/sin,[d,e] 97-ara/jad,[d,e]
		0.493	−0.6	14-tyr,[c]52-jac,[c,e] i, 96-zab/ruz[h]					85-eas/woo-1,[f,g] 96-zab/ruz[h]
		0.494	−0.8	44-sch,[d,e] 52-gab/poi,[d,e] i, 96-zab/ruz[h]			0.648	−1.2	92-miy/tam,[e]93-nak/chu,[e]
		0.495	−1.0	71-ric/rog,[c]82-tak/ter,[d,e]					93-nak/chu-1,[e]
				84-tak/ter,[d]i, 96-zab/ruz[h]					94-tam/mur,[e]i, 96-zab/ruz[h]
296.95	0.500 ± 0.001	0.504	−0.8	46-pel/gal,[d]i, 96-zab/ruz[h]			0.651	−1.7	77-kaw/ohn,[d,e] 85-eas/woo-1,[f,g]
298.15	0.503 ± 0.001	0.505	−0.4	47-wil,[d]i, 96-zab/ruz[h]					96-zab/ruz[h]
		0.506	−0.6	95-nik/jad,[d,e] i, 96-zab/ruz[h]			0.652	−1.8	94-pal/sin,[d,e] 95-ami/gop,[d,e] i,
		0.507	−0.8	88-tak/ter,[d]i, 96-zab/ruz[h]					96-zab/ruz[h]
		0.508	−1.0	54-gab/poi,[d,e] i, 96-zab/ruz[h]			0.652	−1.8	92-miy/tam,[d]93-nak/chu,[d]
298.35	0.504 ± 0.001	0.508	−0.8	53-par/bak,[d]i, 96-zab/ruz[h]					93-nak/chu-1,[d]
301.15	0.511 ± 0.001	0.516	−1.0	62-red/sub,[d]i, 96-zab/ruz[h]					94-tam/mur,[d]85-eas/woo-1,[f,g]
		0.522	−2.1	62-red/sub,[e]i, 96-zab/ruz[h]					96-zab/ruz[h]
303.15	0.517 ± 0.001	0.513	0.8	86-red,[d,e] i, 96-zab/ruz[h]			0.655	−2.3	97-miy/nak[c]
		0.521	−0.8	14-tyr[c]			0.656	−2.4	95-ami/gop,[d,e] 85-eas/woo-1,[f,g]
		0.522	−1.0	88-tak/ter,[d]95-kri/ram,[d,e] 95-nik/jad,[d,e]					96-zab/ruz[h]
				i, 96-zab/ruz[h]	303.15	0.660 ± 0.006	0.638	3.4	76-zel/dya,[d,e] i, 96-zab/ruz[h]
		0.523	−1.1	85-jay/red,[c]65-cop/bey,[d]82-tak/ter,[d,e]			0.643	2.6	76-zel/dya,[d,e] 85-eas/woo-1,[f,g]
				84-tak/ter,[d]					96-zab/ruz[h]
				84-jas/dun,[d]88-ram/sur,[d,e] i, 96-zab/ruz[h]			0.649	1.7	99-ven/rao,[d,e] i, 96-zab/ruz[h]
		0.528	−2.1	90-ven/bab,[d,e] i, 96-zab/ruz[h]			0.657	0.5	99-ven/rao,[d,e] 85-eas/woo-1,[f,g]
308.15	0.530 ± 0.001	0.537	−1.3	85-raj/ram,[d,e] i, 96-zab/ruz[h]					96-zab/ruz[h]
313.15	0.545 ± 0.001	0.549	−0.7	14-tyr[c]			0.665	−0.8	87-raj/red,[d,e] 95-osw/pat-1,[d,e]
		0.550	−0.9	86-red,[d,e] i, 96-zab/ruz[h]					00-osw/pat,[d,e] i
		0.553	−1.4	82-tak/ter,[d,e] 84-tak/ter,[d]i, 96-zab/ruz[h]					96-zab/ruz[h]
		0.554	−1.6	65-cop/bey,[d]i, 96-zab/ruz[h],e i, 96-zab/ruz[h]			0.669	−1.3	87-raj/red,[d,e], 95-osw/pat-1,[d,e]
		0.555	−1.8	84-jas/dun,[d]i, 96-zab/ruz[h]					00-osw/pat,[d,e]
		0.598	−8.9	85-jay/red[c]					85-eas/woo-1,[f,g] 96-zab/ruz[h]
323.15	0.575 ± 0.001	0.587	−2.0	65-cop/bey,[d]84-jas/dun,[d]i, 96-zab/ruz[h]	308.15	0.685 ± 0.007	0.690	−0.7	77-kaw/ohn,[d,e] i, 96-zab/ruz[h]
333.15	0.607 ± 0.002	0.622	−2.4	65-cop/bey,[d]i, 96-zab/ruz[h]			0.694	−1.3	77-kaw/ohn,[d,e] 85-eas/woo-1,[f,g]
343.15	0.642 ± 0.002	0.660	−2.7	65-cop/bey,[d]i, 96-zab/ruz[h]					96-zab/ruz[h]
				Formamide	313.15	0.716 ± 0.008	0.673	6.4	76-zel/dya,[d,e] i, 96-zab/ruz[h]
293.15	0.398 ± 0.001	0.372	7.0	64-mik/roz,[d]69-dun/sto,[f,g] 01-zab/ruz[h]			0.677	5.8	76-zel/dya,[d,e] 85-eas/woo-1,[f,g]
		0.374	6.4	64-mik/roz,[d]i, 01-zab/ruz[h]					96-zab/ruz[h]
296.10	0.401 ± 0.001	0.381	5.2	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]					*N*,*N*-Dimethylacetamide
		0.382	5.0	84-goo/whi,[d,e] i, 01-zab/ruz[h]	298.15	0.645 ± 0.002	0.639	0.9	91-ino/oga[c]
298.15	0.403 ± 0.002	0.398	1.3	47-wil,[d]69-dun/sto,[f,g] i, 01-zab/ruz[h]			0.648	−0.5	98-ami/pat,[d,e] i, 96-zab/ruz[h]
		0.403	0.0	86-bot/bre[c]			0.652	−1.1	77-kaw/ohn,[d,e] i, 96-zab/ruz[h]
		0.411	−1.9	69-dun/sto[c]			0.655	−1.5	95-ami/gop,[d,e] 97-ara/jad,[d,e] i,
300.30	0.405 ± 0.002	0.389	4.1	84-goo/whi,[d,e] i, 01-zab/ruz[h]					96-zab/ruz[h]
		0.390	3.8	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]			0.657	−1.8	91-ino/oga,[d,e] 94-pal/sin,[d,e] i,
303.70	0.409 ± 0.002	0.392	4.3	84-goo/whi,[d,e] i, 01-zab/ruz[h]					96-zab/ruz[h]
		0.394	3.8	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]			0.661	−2.4	77-oba/mur[c]
306.90	0.414 ± 0.002	0.401	3.2	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]	303.15	-	0.667		01-sek/ven,[d,e] i, 96-zab/ruz[h]
		0.398	4.0	84-goo/whi,[d,e] i, 01-zab/ruz[h]			0.675		95-osw/pat-1,[d,e] 00-osw/pat,[d,e] i,
309.90	0.418 ± 0.002	0.402	4.0	84-goo/whi,[d,e] i, 01-zab/ruz[h]					96-zab/ruz[h]
		0.407	2.7	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]	308.15	-	0.699		77-kaw/ohn,[d,e] i, 96-zab/ruz[h]
316.80	0.429 ± 0.002	0.406	5.7	84-goo/whi,[d,e] i, 01-zab/ruz[h]					1-Methylpyrrolidin-2-one
		0.414	3.6	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]	298.15	0.525 ± 0.003	0.535	−1.9	94-pal/sin,[d,e] 84-mur/rod,[f,g]
319.50	0.433 ± 0.003	0.409	5.9	84-goo/whi,[d,e] i, 01-zab/ruz[h]					96-zab/ruz[h]
		0.419	3.3	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]			0.565	−7.1	94-pal/sin,[d,e] 89-mel/sch,[f,g]
326.90	0.448[n]	0.419	6.9	84-goo/whi,[d,e] i, 01-zab/ruz[h]					96-zab/ruz[h]
		0.433	3.5	84-goo/whi,[d,e] 69-dun/sto,[f,g] 01-zab/ruz[h]					

Table 5. (Continued)

T/K	β_T/GPa^{-1} eq 1[a]	β_T/GPa^{-1} lit.	$\delta\beta_T$/%[b]	ref(s)
		2,2,2-Trifluoroethanol		
293.15	1.194 ± 0.004	1.174	1.7	92-tak/nog,[d]i, 96-zab/ruz[h,m]
		1.175	1.6	67-mar,[e]i, 96-zab/ruz[h,m]
298.15	1.240 ± 0.004	1.225	1.2	92-tak/nog,[d,e] i, 96-zab/ruz[h]
		1.228	1.0	92-miy/tam-1,[d,e] i, 96-zab/ruz[h]
		1.229	0.9	81-pat/ali,[e]93-nak/chu-1,[d,e] i, 96-zab/ruz[h]
		1.232	0.6	81-pat/ali,[d]i, 96-zab/ruz[h]
303.15	1.287 ± 0.005	1.279	0.6	92-tak/nog,[d]i, 96-zab/ruz[h,m]
		2,2,3,3,3-Pentafluoropropanol		
298.15	1.274 ± 0.006	1.371	−7.1	92-tak/nog,[e,h] 96-nak/sak,[f,g]
		1.375	−7.3	92-tak/nog[c]
		1.376	−7.4	92-tak/nog,[d,h] 96-nak/sak,[f,g]
		2,2,3,3-Tetrafluoropropanol		
298.15	0.788 ± 0.007	0.771	2.2	92-tak/nog[c]
		0.836	−5.7	92-tak/nog,[d,h] 96-nak/sak,[f,g]
		2,2,2-Trichloroethanol		
303.15	0.678 ± 0.010	0.638	6.3	98-meh/sha[c]
		0.684	−0.9	98-meh/sha,[d,e,h] 97-jen/san[f,g]
		Tetramethylstannane		
293.15	1.546 ± 0.001	1.557	−0.7	80-keh/vog[c]
		1.572	−1.7	80-keh/vog,[d]90-pol/wei,[f,g] 96-zab/ruz[h]
		1.583	−2.3	80-keh/vog,[d]77-ahm/dix,[f,g] 96-zab/ruz[h]
		1.586	−2.5	80-keh/vog,[e]77-ahm/dix,[f,g] 96-zab/ruz[h]
		1.593	−3.0	80-keh/vog,[e]90-pol/wei,[f,g] 96-zab/ruz[h]
298.15	1.616 ± 0.001	1.582	2.1	78-phi/del,[c]84-rie/del[c]
		1.641	−1.5	80-keh/vog,[d]90-pol/wei,[f,g] 96-zab/ruz[h]
		1.662	−2.8	80-keh/vog,[e]90-pol/wei,[f,g] 96-zab/ruz[h]
		1.663	−2.8	80-keh/vog,[d]77-ahm/dix,[f,g] 96-zab/ruz[h]
		1.665	−2.9	80-keh/vog,[e]77-ahm/dix,[f,g] 96-zab/ruz[h]
303.15	1.690 ± 0.001	1.715	−1.5	80-keh/vog,[d]90-pol/wei,[f,g] 96-zab/ruz[h]
		1.736	−2.6	80-keh/vog,[e]90-pol/wei,[f,g] 96-zab/ruz[h]
		1.749	−3.4	80-keh/vog,[d]77-ahm/dix,[f,g] 96-zab/ruz[h]
		1.751	−3.5	80-keh/vog,[e]77-ahm/dix,[f,g] 96-zab/ruz[h]
		Tetramethylsilane		
224.86	1.275 ± 0.018	1.363	−6.5	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.384	−7.9	94-mcl/bar[c]
226.70	1.300 ± 0.018	1.385	−6.1	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.404	−7.4	94-mcl/bar[c]
232.67	1.384 ± 0.017	1.462	−5.3	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.474	−6.1	94-mcl/bar[c]
235.79	1.431 ± 0.016	1.504	−4.9	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.513	−5.4	94-mcl/bar[c]
240.08	1.498 ± 0.015	1.564	−4.2	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.570	−4.6	94-mcl/bar[c]
247.55	1.626 ± 0.015	1.678	−3.1	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.682	−3.3	94-mcl/bar[c]
252.99	1.727 ± 0.014	1.767	−2.3	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.774	−2.6	94-mcl/bar[c]
254.05	1.748 ± 0.014	1.785	−2.1	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.792	−2.5	94-mcl/bar[c]
260.25	1.875 ± 0.013	1.897	−1.2	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		1.910	−1.8	94-mcl/bar[c]
264.71	1.974 ± 0.013	1.983	−0.5	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		2.003	−1.4	94-mcl/bar[c]
268.61	2.066 ± 0.013	2.063	0.1	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		2.091	−1.2	94-mcl/bar[c]
273.28	2.183 ± 0.013	2.165	0.8	94-mcl/bar,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		2.205	−1.0	94-mcl/bar[c]
283.15	2.457 ± 0.014	2.401	2.3	89-tak/ter,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
293.15	2.781 ± 0.016	2.699	3.0	89-tak/ter,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
298.15	2.961 ± 0.017	2.860	3.5	89-tak/ter,[d]89-bao/cac,[f,g] 96-zab/ruz[h]
		Tetraethylsilane		
283.15	0.991 ± 0.004	1.016	−2.5	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
293.15	1.061 ± 0.004	1.076	−1.4	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
		1.082	−1.9	80-keh/vog,[d,e] 90-yok/tak,[f,g] 96-zab/ruz[h]
		1.083	−2.0	80-keh/vog[c]
298.15	1.100 ± 0.004	1.107	−0.6	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
		1.112	−1.1	80-keh/vog,[d,e] 90-yok/tak,[f,g] 96-zab/ruz[h]
303.15	1.140 ± 0.005	1.139	0.1	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
313.15	1.227 ± 0.006	1.209	1.5	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
323.15	1.323 ± 0.006	1.307	1.2	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
333.15	1.431 ± 0.007	1.365	4.8	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
283.15	1.078 ± 0.004	1.072	0.6	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
293.15	1.163 ± 0.004	1.154	0.8	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
298.15	1.209 ± 0.004	1.245	−2.9	78-phi/del[c]
		1.197	1.0	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
303.15	1.257 ± 0.004	1.243	1.1	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
313.15	1.362 ± 0.005	1.340	1.6	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
323.15	1.479 ± 0.006	1.448	2.1	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
333.15	1.611 ± 0.007	1.566	2.9	89-tak/ter,[d]90-yok/tak,[f,g] 96-zab/ruz[h]
		Octamethylcyclotetrasiloxane		
293.15	1.456[n]	1.591	−8.4	58-wat/van,[d]i, 96-zab/ruz[h]
		1.586	−8.2	80-nie/sch,[d]i, 96-zab/ruz[h]
295.15	1.476[n]	1.465	0.8	63-ros/hil,[j]i
		1.491	−1.0	63-ros/hil[c]
		1.610	−8.3	80-nie/sch,[d]i, 96-zab/ruz[h]
297.60	1.502[n]	1.493	0.6	63-ros/hil,[j]i
		1.517	−1.0	63-ros/hil[c]
		1.635	−8.1	80-nie/sch,[d]i, 96-zab/ruz[h]
298.15	1.508[n]	1.499	0.6	63-ros/hil,[j]i
		1.523	−1.0	63-ros/hil[c]
		1.531	−1.5	77-ewi/mar[c]
		1.54	−2.1	61-shi/hil[c]
		1.641	−8.1	80-nie/sch,[d]i, 96-zab/ruz[h]
302.71	1.558[n]	1.553	−0.3	63-ros/hil,[j]i
		1.574	−1.0	63-ros/hil[c]
		1.699	−8.3	80-nie/sch,[d]i, 96-zab/ruz[h]
308.15	1.622[n]	1.775	−8.6	80-nie/sch,[d]i, 96-zab/ruz[h]
308.80	1.630[n]	1.653	−1.4	63-ros/hil,[j]i
		1.669	−2.3	63-ros/hil[c]
		1.785	−8.7	80-nie/sch,[d]i, 96-zab/ruz[h]
317.99	1.747 ± 0.006	1.820	−4.0	63-ros/hil[c]
		Dimethyl Sulfoxide		
293.15	0.518[n]	0.515	0.6	78-zel/dya,[d,e] i, 96-zab/ruz[h]
293.35	0.519[n]	0.510	1.8	69-lau/mal,[j]i
296.65	0.523 ± 0.006	0.517	1.2	69-lau/mal,[j]i
297.15	0.524 ± 0.006	0.525	−0.2	76-cha/mac,[j]i
298.15	0.526 ± 0.006	0.52	1.2	76-cha/mac[c]
		0.522	0.8	65-for/moo,[d,e] i, 96-zab/ruz[h]
		0.523	0.6	75-dac/bir[c]
		0.524	0.4	98-cha/kum,[d,e] i, 96-zab/ruz[h]
		0.525	0.2	71-mac/hyn,[j]i
		0.526	0.0	95-ami/gop,[d,e] 98-ami/pat,[d,e] i, 96-zab/ruz[h]
		0.527	−0.2	92-ara/ami,[d,e] 97-ara/jad,[d,e] 95-ami/gop,[d,e] i, 96-zab/ruz[h]
		0.529	−0.6	92-miy/tam-1,[d,e] 93-nak/chu,[d,e] 94-tam/mur,[d,e] 97-miy/nak,[d,e] 99-nai/ali,[d,e] i, 96-zab/ruz[h]
		0.530	−0.8	78-wer/les,[d,e] i, 96-zab/ruz[h]
		0.531	−0.9	93-das/haz,[d,e] i, 96-zab/ruz[h]
298.65	0.527 ± 0.006	0.530	−0.6	71-mac/hyn,[j]i
299.75	0.528 ± 0.006	0.532	−0.8	69-lau/mal,[j]i
303.15	0.534 ± 0.006	0.530	0.8	78-zel/dya,[d,e] i, 96-zab/ruz[h]
		0.539	−0.9	95-osw/pat-1,[d,e] i, 96-zab/ruz[h]
		0.541	−1.3	92-ara/ami,[d,e] i, 96-zab/ruz[h]
		0.543	−1.7	99-nai/ali,[d,e] i, 96-zab/ruz[h]
303.45	0.534 ± 0.006	0.544	−1.8	69-lau/mal,[j]i
		0.559	−4.5	76-cha/mac,[j]i
308.15	0.542 ± 0.006	0.557	−2.7	92-ara/ami,[d,e] i, 96-zab/ruz[h]
		0.558	−2.9	99-nai/ali,[d,e] i, 96-zab/ruz[h]
309.45	0.544 ± 0.06	0.562	−3.2	69-lau/mal,[j]i
310.05	0.545 ± 0.006	0.564	−3.4	69-lau/mal,[j]i
310.95	0.546 ± 0.006	0.549	−0.5	71-mac/hyn,[j]i
313.15	0.550 ± 0.007	0.545	0.9	78-zel/dya,[e]i, 96-zab/ruz[h]
		0.549	0.2	78-zel/dya,[d]i, 96-zab/ruz[h]
		0.570	−3.5	92-dew/meh-1,[d,e] i, 96-zab/ruz[h]
		0.573	−4.0	99-nai/ali,[d,e] i, 96-zab/ruz[h]
318.15	0.558 ± 0.008	0.591	−5.6	99-nai/ali,[d,e] i, 96-zab/ruz[h]
		0.60	−3.6	76-cha/mac[c]
322.65	0.566 ± 0.008	0.618	−4.2	76-cha/mac,[j]i
324.95	0.571[n]	0.599	−4.7	71-mac/hyn,[j]i
		0.607	−5.9	76-cha/mac,[j]i
330.65	0.581[n]	0.645	−9.9	76-cha/mac,[j]i

[a] Uncertainty is estimated as ±2s, where s is a standard deviation derived from a covariance matrix of each fit. [b] [β_T(eq 1)-β_T(lit)] 100/β_T(lit). [c] Isothermal compressibility, $\beta_T = (1/\rho)\,(\partial\rho/\partial P)_T = -(1/V)(\partial V/\partial P)_T$. [d] Sound speed. [e] Isentropic compressibility, $\beta_S = (1/\rho)\,(\partial\rho/\partial P)_S = -(1/V)(\partial V/\partial P)_S$. [f] Density. [g] Thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$. [h] Isobaric heat capacity. [i] Density and/or thermal expansivity evaluated from a fit of selected density data taken from more than one source. [j] Thermal pressure coefficient, $\gamma_V = (\partial P/\partial T)_V$; β_T was obtained as $\beta_T = \alpha_P/\gamma_V$. [k] Obtained using densimeter and piezometer, respectively [m] Value of heat capacity at T = 298.15 K was used. [n] Extrapolated beyond temperature limits of eq 1.

Table 6. Parameters a_i of Smoothing Functions 12 or 13 Fitted to Selected Density Values, $\rho[T,P = 0.1\ \text{MPa or } P_{sat}(T)]$, Critical Densities,[a] ρ_c, Critical Temperatures, T_c, Temperature Ranges of Density Data, T_{min} and T_{max}, and RMSDs of the Fits

eq	a_0	a_1	a_2	a_3	a_4	a_5	ρ_c / kg·m^{-3}	T_c / K	T_{min} / K	T_{max} / K	RMSD / kg·m^{-3}	ref
					1-Aminopropane							
12	1.957 811	0.987 548	−1.967 087	1.879 882			259.259	497.00	188.39	496.00	0.190	90-cha/gad
					1-Aminobutane							
12	1.921 817	1.015 999	−1.793 001	1.615 440			264.036	531.90	224.05	531.00	0.235	93-das/fre
					2-Methyl-2-propanamine							
12	1.663 549	1.520 586	−2.521 972	3.724 154	−1.616 855		250.473	483.90	206.20	483.00	0.316	93-das/fre
					1-Aminopentane							
12	5.494 614	−11.684 60	13.867 142	−4.810 753			254.125[b]	553.90[c]	223.15	423.15	0.552	86-trc
					Aminobenzene							
12	2.323 597	1.401 463	−6.017 565	5.828 077	1.303 453	−2.068 705	332.602	699.00	267.13	698.00	0.216	90-cha/gad
					2-Methyl-1-aminobenzene							
12	1.691 182	0.606 118	0.293 326	0.190 586			321.788	707.00	256.80	706.00	0.252	90-cha/gad
					4-Methyl-1-aminobenzene							
12	1.730 166	0.591 646	0.295 498	0.196 531			315.163	706.00	316.90	705.00	0.326	90-cha/gad
					Ethanenitrile							
12	3.319 763	−7.966 222	22.355 211	−24.088 40	10.008 734		237.298[c]	545.50[c]	233.45	523.30	0.272	75-fra/fra, 85-kra/mue
					Ethanenitrile-d_3							
13	983.898 74	8.097 200	−19.955 56						303.15	363.15	0.000[d]	77-sch/sch
					Propanenitrile							
12	10.096 843	−51.158 87	120.754 42	−121.136 8	45.110 512		240.522[c]	561.30[c]	190.36	467.55[e,f]	0.142	84-sha/gus
					Butanenitrile							
12	2.857 821	−9.613 227	32.385 023	−38.628 62	16.469 494		242.479[c]	585.40[c]	176.94	490.46[e,g]	0.310	84-sha/gus
					2-Methylpropenenitrile							
13	1158.482 9	−122.581 5							293.00	373.00[e,h]	0.423	83-gus/naz
					Benzonitrile							
12	14.596 031	−50.449 85	68.653 071	−30.128 55			301.532[c]	699.40[c]	290.00	523.00[e,i]	0.909	78-gus/naz, 86-gus
					Pyridine							
12	1.999 947	0.890 974	−1.851 331	1.875 984			325.521	620.00	231.49	619.00	0.210	93-das/fre
					Piperidine							
12	1.675 910	0.589 116	0.268 956	0.165 816			295.657	594.00	262.12	593.00	0.254	93-das/fre
					1-Azaindene							
12	1.000 294	1.486 565					371.318[c]	803.56[c]	323.15	353.15	0.112	95-yok/ebi
					Quinoline							
12	2.274 707	1.447 414	−4.620 742	3.798 895			348.145	782.00	258.37	781.00	0.299	93-das/fre
					Nitromethane							
12	10.059 166	−19.564 52	13.104 731				352.834[c]	588.00[c]	247.40	308.15	0.424	80-vit/ber, 90-uos/mat-1, 01-tro/tov
					Nitroethane							
12	2.861 827	−2.019 428	2.363 097				329.242[c]	592.00[c]	283.15	363.15	0.361	77-gup/han, 90-uos/mat-1, 00-tro/car
					1-Nitropropane							
13	995.6								298.15	298.15		90-uos/mat-1
					2-Nitropropane							
13	983.7								298.15	298.15		90-uos/mat-1
					2-Methyl-2-nitropropane							
13	1236.283 9	−84.262 38	−3.375 000						313.15	353.15	0.000[j]	96-jen/reu
					Nitrobenzene							
12	4.479 294	−5.728 456	4.394 779				362.093[c]	718.00[c]	273.15	373.15	0.319	14-tyr, 39-gib/loe-1, 60-hil/goc, 79-abd/dzh, 82-tak/ter, 90-uos/mat-1
					Formamide							
12	1.246 017	1.660 539					346.468[c]	773.00[c]	278.94	338.15	0.082	69-dun/sto, 86-bot/bre
					N-Methylformamide							
13	1252.839 6	−85.284 21							288.15	313.15	0.039	85-eas/woo-1
					N,*N*-Dimethylformamide							
13	1172.052 5	−59.967 20	−5.600 000						288.15	313.15	0.000[j]	85-eas/woo-1
					N,*N*-Dimethylacetamide							
13	1191.632 3	−79.255 86	−2.132 163						283.15	343.15	0.230	79-gri/goa, 80-khi/gri, 91-pac
					1-Methoxy-2-nitrobenzene							
13	1254.2								293.15	293.15		60-hil/goc
					1-Methylpyrrolidin-2-one							
13	1210.156 6	−34.246 74	−9.251 797						283.15	333.15	0.368	84-mur/rod
13	1278.283 1	−73.754 41	−3.350 590						253.15	298.15	0.002	89-mel/sch

Table 6. (Continued)

eq	a_0	a_1	a_2	a_3	a_4	a_5	ρ_c / kg·m^{-3}	T_c / K	T_{min} / K	T_{max} / K	RMSD / kg·m^{-3}	ref
					3-Cyanopropanal							
13	1108.718 1	82.590 046	−73.986 39	14.409 592	−1.092 390				290.40	505.00[e,k]	0.309	81-mus/gan
					2-Fluoroethanol							
13	1354.963 6	−57.929 43	−8.841 580						278.15	338.13	0.024	97-woo
					2,2-Difluoroethanol							
13	1621.061 3	−77.470 29	−10.579 75						278.15	338.15	0.041	95-mal/woo
					2,2,2-Trifluoroethanol							
12	1.975 513	0.944 766	−0.292 081				484.000[l]	499.29[l]	263.15	430.627	0.816	89-bae/klo, 90-sve/sid, 92-kab/yam, 92-kab/yam-1, 93-sau/hol, 94-mat/yam, 99-her/oli
					2,2,3,3,3-Pentafluoropropanol							
12	3.086 144	−2.053 610	1.789 255				523.000[m]	497.70[m]	278.54	318.40	0.106	96-nak/sak
13	2106.093 7	−201.152 000							298.15	323.15	0.000[j]	94-mat/yam
					2,2,3,3-Tetrafluoropropanol							
12	1.878 745	0.883 004					495.001[m]	557.20[m]	278.54	328.37	0.239	96-nak/sak
13	1977.296 1	−166.588 000							298.15	323.15	0.000[j]	94-mat/yam
					2,2,2-Trichloroethanol							
13	1885.138 2	−81.695 80	−9.775 200						290.15	355.15	1.034	97-jen/san
					Bis(difluoromethyl) Ether							
12	17.112 497	−100.596 9	252.226 02	−278.196 4	114.876 27		529.000	420.25	273.58	367.37	0.029	92-def/gil
					2,2,2-Trifluoroethyl Difluoromethyl Ether							
13	2543.832 4	−775.201 7	216.079 70	−28.980 64					274.15	338.13[n]	0.063	95-mal/woo-1
12	1.815 682	1.449 995	−1.839 450	1.531 503			515.600	444.03	275.00	370.00		97-def/mol
					Pentafluoroethyl Methyl Ether							
12	2.143 027	−5.487 065	32.463 157	−75.307 81	82.004 440	−33.886 162	509.001[o]	406.83[o]	259.98	404.25	0.416	01-oht/mor, 01-wid/tsu
					1,2,2,2-Tetrafluoroethyl Difluoromethyl Ether							
12	2.119 506	0.230 471	0.605 628				533.000[p]	428.95[p]	274.15	338.13[q]	0.072	95-mal/woo-1
					Heptafluoropropyl Methyl Ether							
12	1.839 776	0.686 292	0.057 145	0.250 296			530.001	437.70	249.98	435.11	0.542	01-oht/mor, 01-wid/uch
					Pentafluorobenzonitrile							
13	2085.724 6	−170.701 0							283.20	363.20	0.002	90-pol/wei
					Tetramethylstannane							
13	1851.014 1	−181.396 3							267.40	366.90	0.002	90-pol/wei
13	1606.343 3	−33.424 29	−24.275 08						273.15	323.18	0.175	77-ahm/dix
					Tetramethylsilane							
12	5.245 941	−13.198 68	18.122 199	−7.568 344			244.390[r]	448.64[r]	198.16	342.18	0.485	89-bao/cac, 90-yok/tak
					Tetraethylsilane							
12	7.429 032	−14.964 80	10.243 597				293.358[c]	603.70[c]	283.15	336.55	0.210	90-yok/tak
					Hexamethyldisilane							
13	−257.364 3	675.515 40	−117.350 0						303.20	323.20	0.000[i]	82-bri/wue
					Tetraethoxysilane							
12	4.181 934	−5.966 881	4.748 205				317.093[c]	592.20[c]	283.13	333.31	0.160	90-yok/tak
					Octamethylcyclotetrasiloxane							
12	1.152 753	5.090 081	−7.557 288	4.611 995			301.441[s]	586.00[s]	292.06	413.17	0.256	68-mar, 76-ben/win, 84-eas/woo, 94-mcl/bar-1
12	2.906 627	−2.200 901	2.502 712				301.441[s]	586.00[s]	313.14	413.17	0.057	76-ben/win, 84-eas/woo
					Dimethyl Sulfoxide							
12	0.833 186	1.722 722					375.652[c]	738.00[c]	293.60	323.00	0.803	80-fuc/ghe
12	2.175 588	−1.998 848	2.517 888				375.652[c]	738.00[c]	292.23	398.15	0.162	22 various sources

[a] Critical densities are given with three decimal places, since they were calculated from rounded values of critical molar volumes in some cases. [b] Estimated by the Lydersen method. [c] From database [93-cda]. [d] Interpolation using values obtained by extrapolation from elevated pressures to 0.1 MPa. [e] Densities were obtained by extrapolation of values at elevated pressures to saturated vapor pressure. [f] Extrapolated values for T > 368.19 K. [g] Extrapolated values for T > 390.62 K. [h] Extrapolated values for T > 353 K. [i] Extrapolated values for T > 473 K. [j] Interpolation. [k] Extrapolated values for T > 333.75 K, extrapolation to 0.1 MPa. [l] From [93-sau/hol]. [m] From [92-tak/nog]. [n] Values for T > 293.15 K were estimated by the modified Rackett method [85-cam/tho] using experimental density values at 274.15 and 293.15 K and critical parameters from [98-goo/def]. [o] From [01-oht/mor, 01-yos/miz]. [p] From [96-sak/sat]. [q] Values for T > 288.15 K were estimated by the modified Rackett method [85-cam/tho] using experimental density values at 274.15 and 288.15 K and critical parameters from [96-sak/sat]. [r] From [77-mcg/mck]. [s] From [01-nov].

Table 7. Parameters a_i of Smoothing Function 14, Critical Temperatures, T_c, Critical Pressures, P_c,Temperature Ranges of Saturated Vapor Pressure Data, T_{min} and T_{Max}, and Relative Standard Deviations, δP_s

a_0	a_1	a_2	a_3	T_c / K	P_c / MPa	T_{min} / K	T_{max} / K	δP_s / %	ref
2-Methylpropenenitrile[a]									
Bis(difluoromethyl) Ether									
−8.884 543	5.133 985	−7.856 370	2.832 724	420.25	4.228	279.00	420.00	0.01	92-def/gil
Pentafuoroethyl Methyl Ether									
−7.771 214	1.735 502	−2.371 910	−10.938 413	406.83	2.887	259.98	406.15	0.10	01-oht/mor, 01-wid/tsu
1,2,2,2-Tetrafluoroethyl Difluoromethyl Ether									
−8.133 251	2.101 659	−3.556 315	−5.050 692	428.95[b]	3.050[b]	269.15	428.95		*c*
Heptafluoropropyl Methyl Ether									
−7.997 881	1.820 040	−2.952 480	−10.592 214	437.70	2.476	299.99	437.50	0.14	01-oht/mor, 01-wid/uch
Tetramethylstannane									
−7.406 272	1.790 803	−2.710 780	−3.249 246	521.81[d]	2.981[d]	273.25	520.67	0.38	30-bul/hau, 36-tho/lin, 78-hug/mcg
Tetramethylsilane									
−7.258 475	1.817 999	−2.394 098	−2.870 613	448.64[e]	2.821[e]	208.98	448.58	0.89	41-ast/ken, 53-tan/kay, 76-hic/you, 77-mcg/mck

[a] Antoine equation $\ln(P/\text{kPa}) = 14.1148664 - 2970.78355/(T/\text{K} - 50.602)$ evaluated from data [48-pet/mar] in the range from 273.15 to 373.15 K was employed. [b] From [96-sak/sat]. [c] Fit of values estimated by the Riedel method [54-rie] using critical parameters from [96-sak/sat] and the normal boiling point temperature from [98-mat/tan]. [d] From [78-hug/mcg]. [e] From [77-mcg/mck].

The isothermal compressibility calculated from the fit of data [90-uos/mat] for 2-methylpropanenitrile is $\beta_T(T = 298.15\ \text{K}, P = 0.1\ \text{MPa}) = 1.139\ \text{GPa}^{-1}$. No data for a comparison were available, as well as for 2-methylpropenenitrile. It is worthy of mention that the value of the parameter c_0 (Table 3) for 2-methylpropenenitrile is unusually large.

Four data sets were available for benzonitrile. Two of them [90-uos/mat, 01-tak/fuj] present data along the isotherm 298.15 K, and their pressure ranges overlap. Separate fits of these two sets resulted in $c_0 = 0.095\ 664$, $b_0 = 151.6381$ MPa, $T_{min} = T_{max} = 298.15$ K, $P_{min} = 1.66$ MPa, $P_{max} = 150.00$ MPa, RMSD = 0.246 kg·m^{-3}, and $\text{RMSD}_r = 0.024\%$. The isothermal compressibility calculated from the fit $\beta_T(T = 298.15\ \text{K}, P = 0.1\ \text{MPa}) = 0.630\ \text{GPa}^{-1}$ deviates by −1.6% from the average literature value (0.640 GPa^{-1}, Table 5). The other two sets [78-gus/naz, 86-gus] deviate from the data [90-uos/mat, 01-tak/fuj], and therefore the data points [78-gus/naz] retained for the final fit (Table 3) were those for higher temperatures only. The point of inflection appears on the $B(T)$ curve at $T = 388$ K, which indicates an inconsistency of the retained data sets. Deviations of isothermal compressibilities calculated from the fit from literature values are negative and slightly increase with increasing temperature (Table 5). Extrapolation toward lower temperatures leads to positive deviations in isothermal compressibilities.

The isothermal compressibility calculated from the fit of the data [90-uos/mat] for phenylethanenitrile is $\beta_T(T = 298.15\ \text{K}, P = 0.1\ \text{MPa}) = 0.465\ \text{GPa}^{-1}$. No data for a comparison were available.

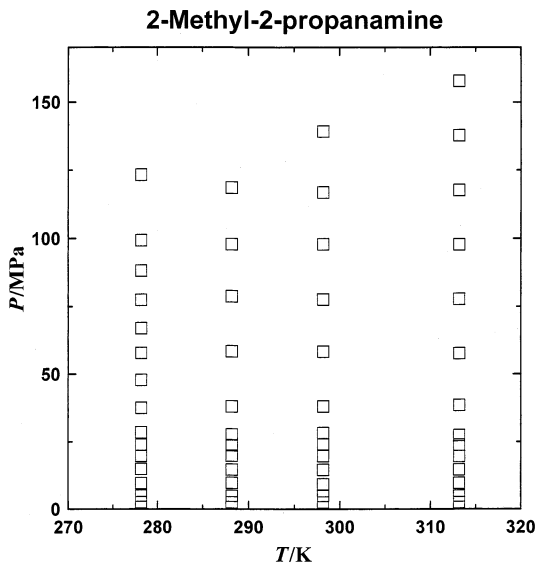
Heterocyclic C−H−N Compounds. The final fit for pyridine (Table 3) represents predominantly smoothed values [79-fur/mun]. The uncertainty of the original experimental data is rather large (4 kg·m^{-3}), as declared by the authors [79-fur/mun]. The RMSD of the fit is much smaller, obviously because of the fact that the smoothed values were fitted. The calculated isothermal compressibilities are systematically lower than the data from the literature (average deviation −4.5%, including extrapolated values, see Table 5).

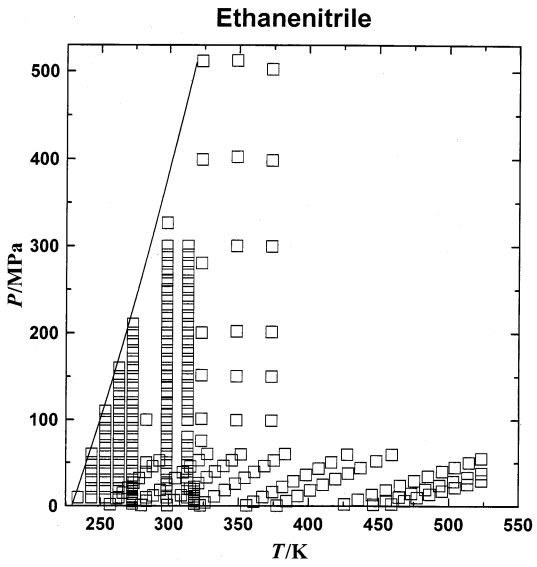
One data set was available for 1-azaindene at $T = 333.15$ K. The isothermal compressibility calculated from the fit is $\beta_T(T = 333.15\ \text{K}, P = 0.1\ \text{MPa}) = 0.509\ \text{GPa}^{-1}$. No data were available for a comparison.

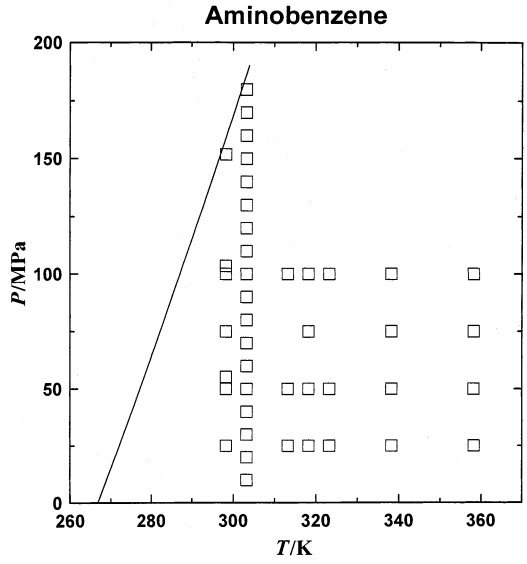
A tentative correlation of all data points available for quinoline resulted in the fit with two inflection points on the $B(T)$ curve (at 423 and 440 K) and the deviations of calculated isothermal compressibilities from literature values (Table 5) −9.1% (298.55 K), −7.1% (303.15 K), and −4.1% (313.15 K). The fit of the data [88-sid/tej] resulted in even lower values of isothermal compressibility. A separate fit of the data [96-cha/lee, 96-cha/lee-1] [$c_0 = 0.059\ 029$, $b_0 = 93.3176$ MPa, $b_1 = -49.7806$ MPa·K^{-1}, $b_2 = 5.3620$ MPa·K^{-2}, $T_0 = 353.15$ K, $T_{min} = 298.15$ K, $T_{max} = 413.15$ K, $P_{min} = 1.00$ MPa, $P_{max} = 30.00$ MPa, RMSD = 0.105 kg·m^{-3}, $\text{RMSD}_r = 0.010\%$, bias = −0.044 kg·m^{-3}, $N_p = 63$, $\pm = -25$, $s_w = 0.474$] yields isothermal compressibilities at 0.1 MPa: $\beta_T(T = 298.55\ \text{K}) = 0.483\ \text{GPa}^{-1}$, $\beta_T(T = 303.15\ \text{K}) = 0.493\ \text{GPa}^{-1}$, and $\beta_T(T = 313.15\ \text{K}) = 0.517\ \text{GPa}^{-1}$, which are in excellent agreement with literature data (Table 5). The data [96-ran/eat] are not consistent with the data [96-cha/lee-1] in the overlapping T and P intervals, and therefore only high-temperature data [96-ran/eat] were retained in the final fit (Table 3). The representation of data [96-cha/lee, 96-cha/lee-1] is, however, affected, and the agreement in isothermal compressibilities is worse (Table 5).

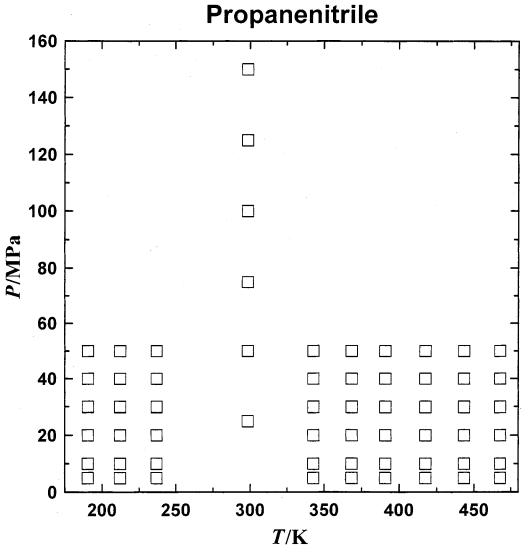
C−H−O−N Compounds. Nitro Compounds. Two data sets per substance were available for nitromethane and nitroethane [77-gup/han, 90-uos/mat-1]. The two sets are mutually in good agreement except for the isotherm $T = 318.15$ K [77-gup/han] of nitromethane that was rejected from the final fit. The isothermal compressibilities calculated from the fit for nitromethane are in very good agreement with the values from the literature (Table 5); the deviations are mostly below 1%. Rather worse agreement is observed for nitroethane, where the deviations are systematically negative (2.2% on the average).

One source of $P-\rho-T$ data [90-uos-mat-1] was available for 1-nitropropane and 2-nitropropane. A comparison of the fits with isothermal compressibilities taken from the literature resulted in the deviations −0.7% and −4.7%, respectively (Table 5). A conclusion is, however, difficult to make, since the values used for the comparison were taken from one source only [88-dew/sha]. It should be noted that isothermal compressibilities taken from [88-dew/sha] for nitromethane and nitroethane exhibit positive deviations from other literature data.


2-Methyl-2-propanamine
P/MPa
T/K
0
50
100
150
270
280
290
300
310
320


Ethanenitrile
P/MPa
T/K
0
100
200
300
400
500
250
300
350
400
450
500
550


Aminobenzene
P/MPa
T/K
0
50
100
150
200
260
280
300
320
340
360


Propanenitrile
P/MPa
T/K
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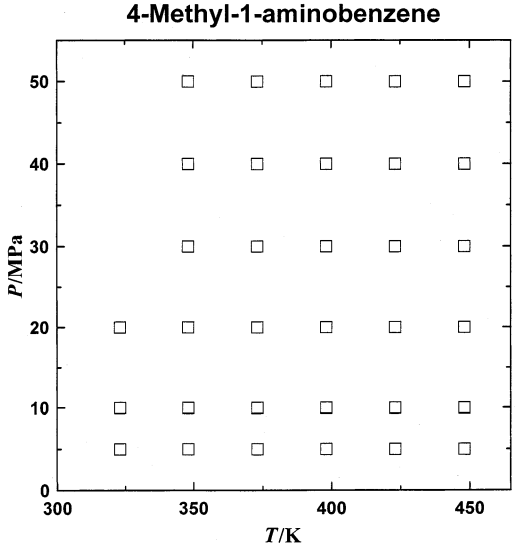
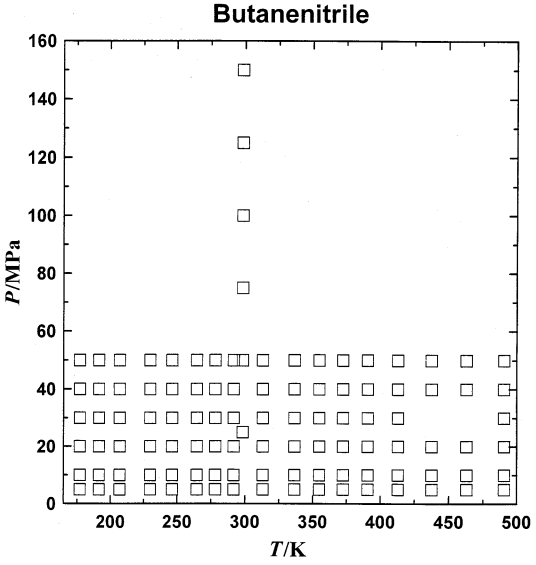
40
60
80
100
120
140
160
200
250
300
350
400
450


4-Methyl-1-aminobenzene
P/MPa
T/K
0
10
20
30
40
50
300
350
400
450


Butanenitrile
P/MPa
T/K
0
20
40
60
80
100
120
140
160
200
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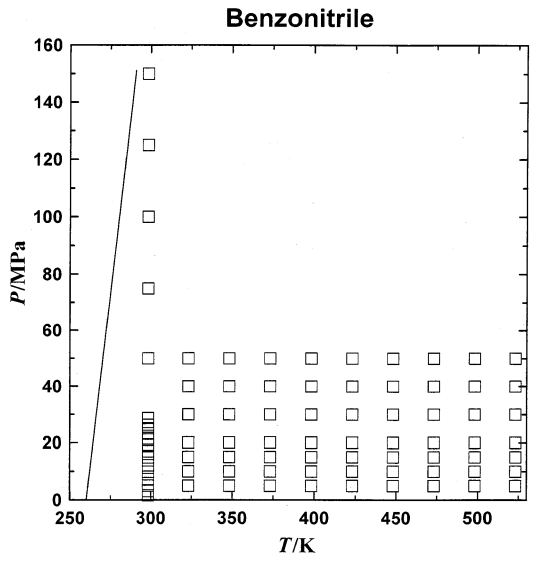
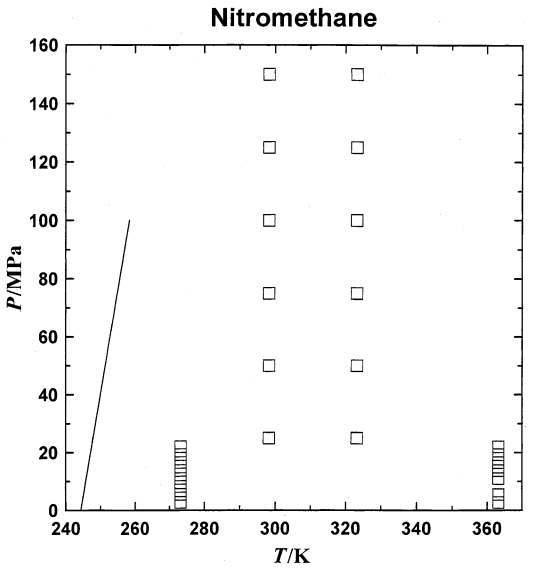
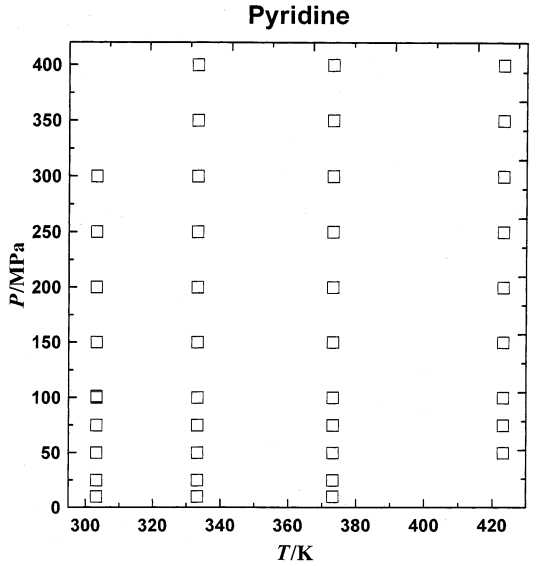
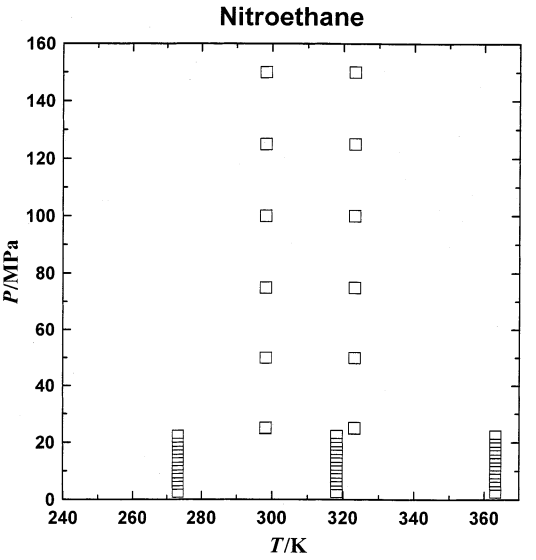
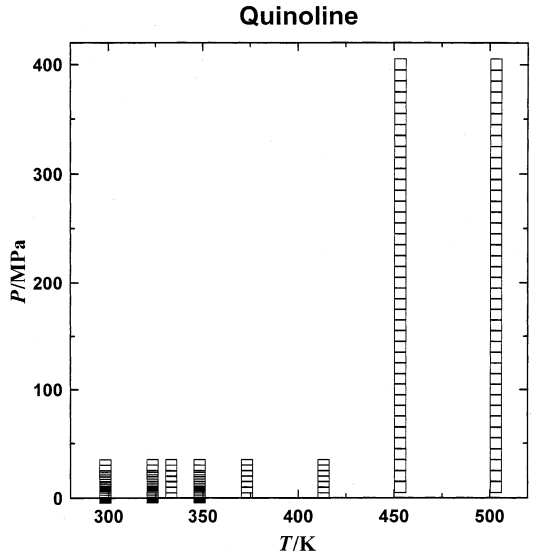
400
450
500

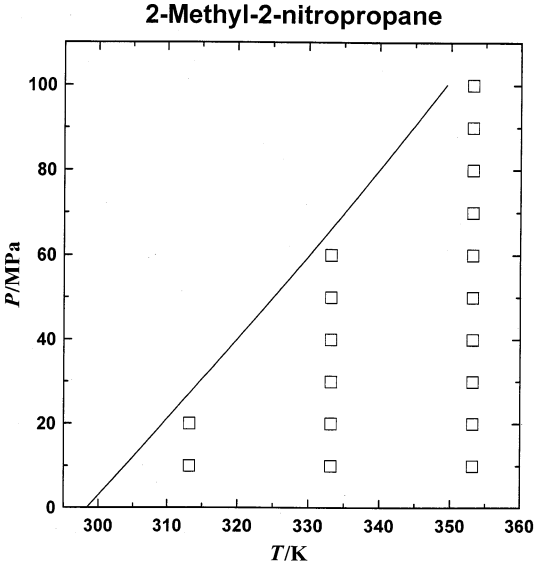

Benzonitrile
P/MPa
T/K

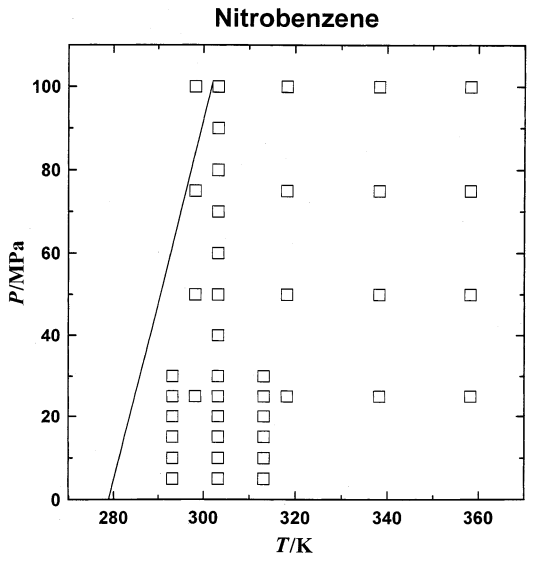

Nitromethane
P/MPa
T/K

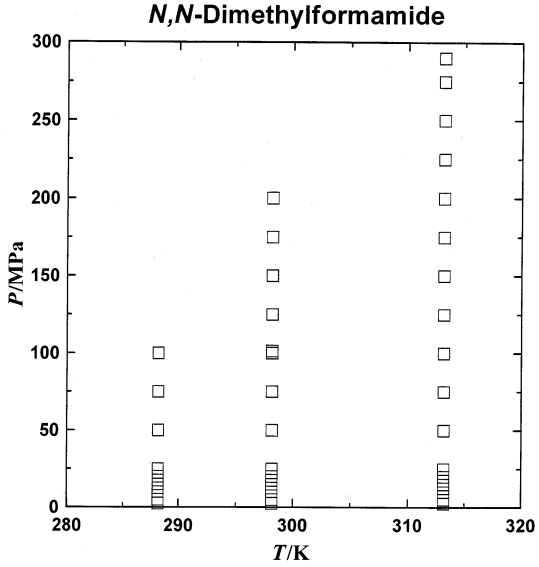

Pyridine
P/MPa
T/K

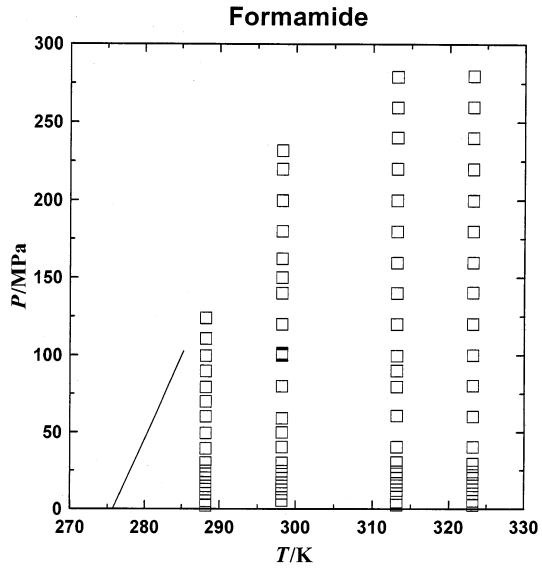

Nitroethane
P/MPa
T/K

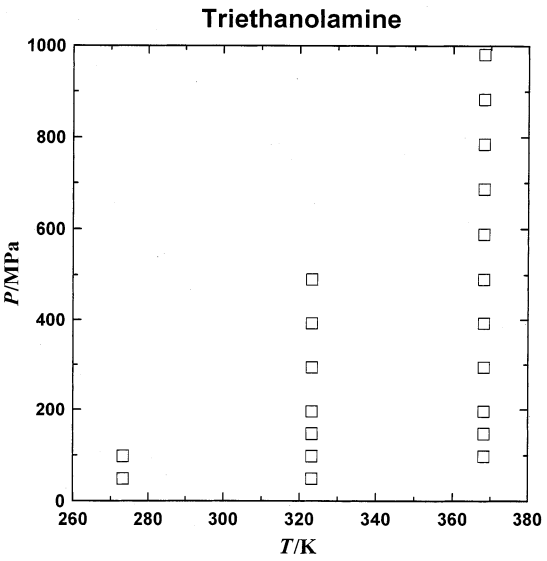

Quinoline
P/MPa
T/K

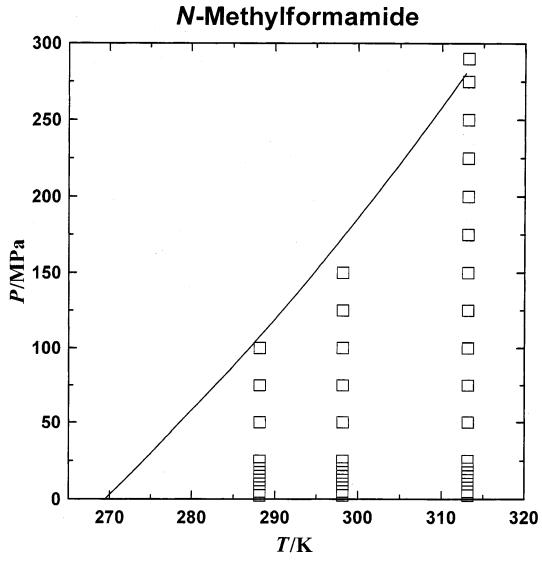

2-Methyl-2-nitropropane
P/MPa
T/K

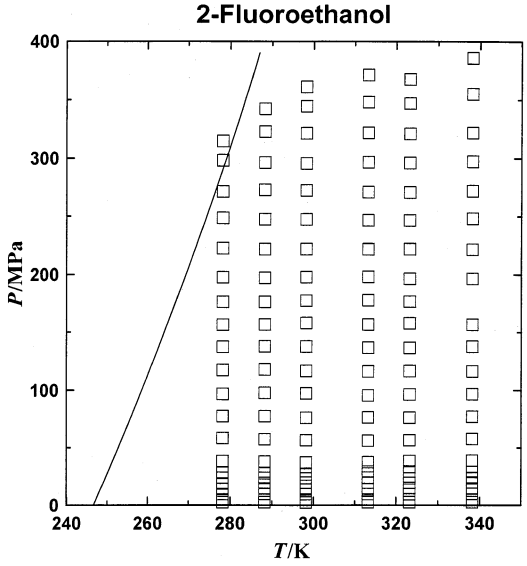

Nitrobenzene
P/MPa
T/K

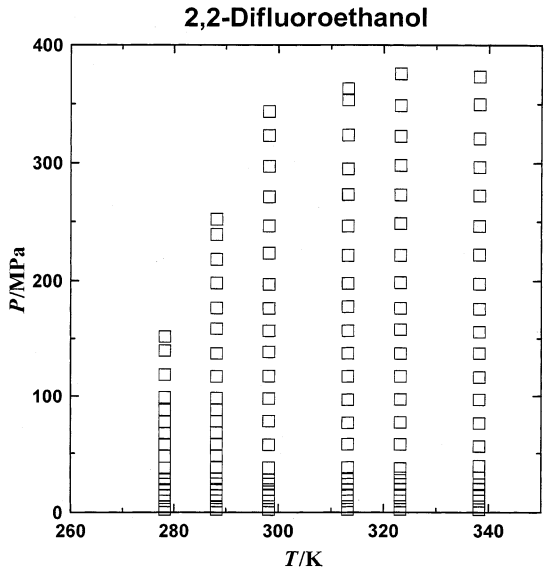

N,N-Dimethylformamide
P/MPa
T/K

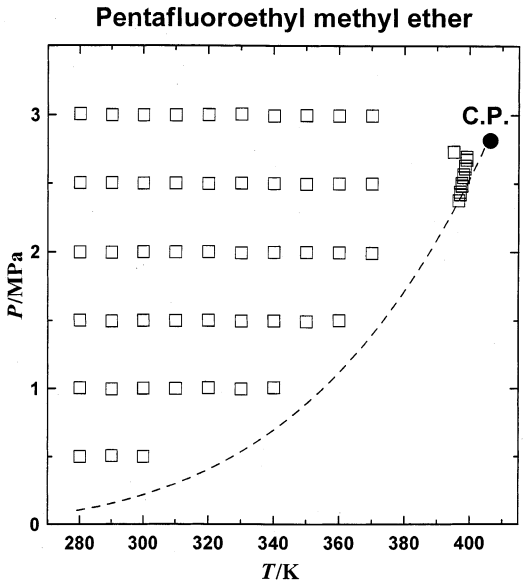

Formamide
P/MPa
T/K

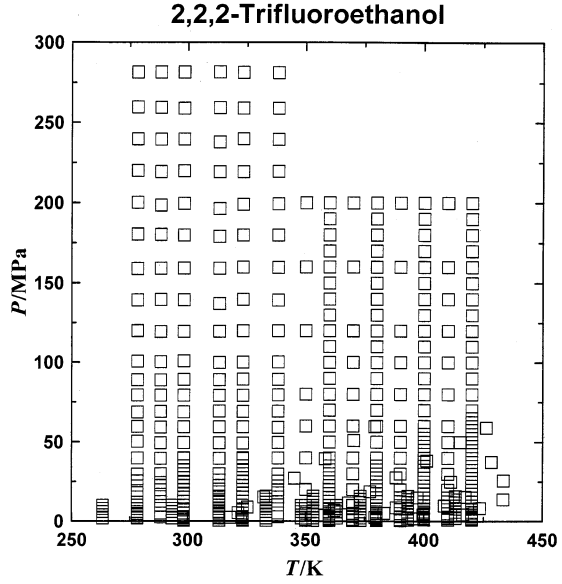

Triethanolamine
P/MPa
T/K

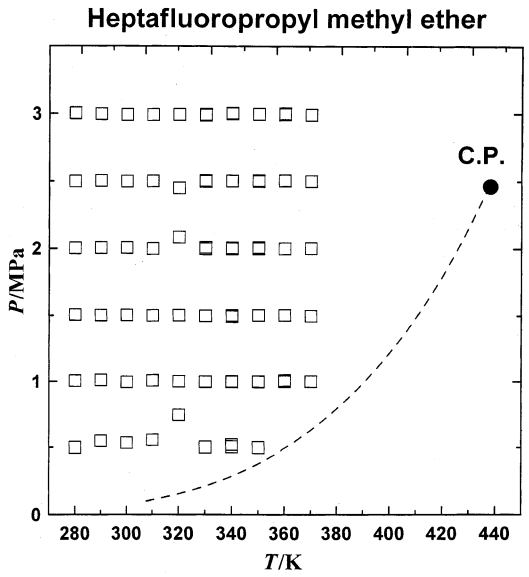

N-Methylformamide
P/MPa
T/K

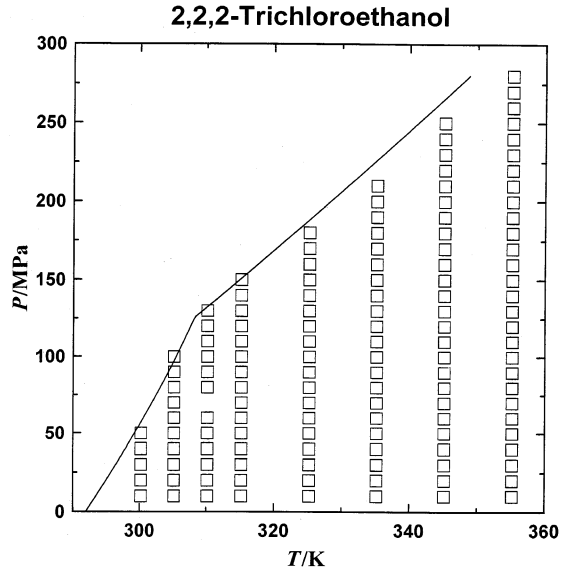

2-Fluoroethanol
P/MPa
T/K

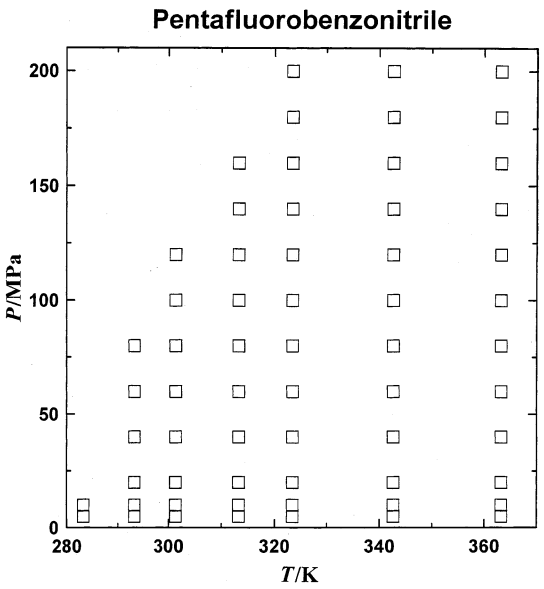

2,2-Difluoroethanol
P/MPa
T/K


Pentafluoroethyl methyl ether
C.P.
P/MPa
T/K


2,2,2-Trifluoroethanol
P/MPa
T/K


Heptafluoropropyl methyl ether
C.P.
P/MPa
T/K


2,2,2-Trichloroethanol
P/MPa
T/K


Pentafluorobenzonitrile
P/MPa
T/K

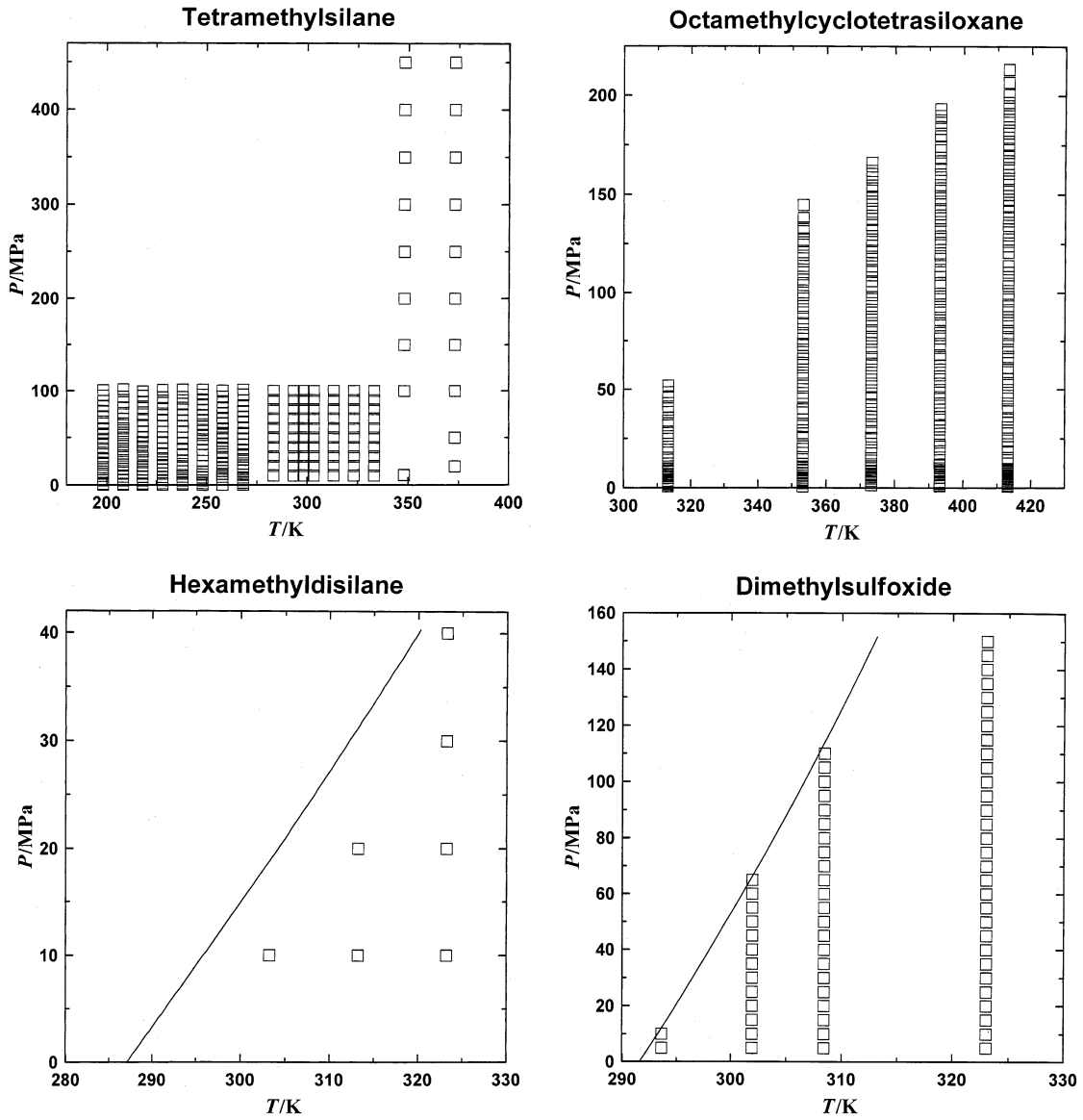


Figure 1. Temperature and pressure coordinates of data points retained in the correlations for the fits in Table 3 where $P-T$ areas of retained data points are not rectangular. Solid−liquid equilibrium curves (full lines) represent smoothed experimental data (generated from the Simon equation) taken mostly from [63-bab] except for 2-methyl-2-nitropropane [96-jen/reu], *N*-methylformamide [85-eas/woo-1], 2-fluoroethanol [97-woo], 2,2,2-trichloroethanol [97-jen/san], hexamethyldisilane [82-bri/wue], and dimethyl sulfoxide [80-fuc/ghe]. Vapor−liquid equilibrium curves for pentafluoroethyl methyl ether and heptafluoropropyl methyl ether (dashed lines with critical point, C.P.) correspond to functions presented in Appendix 2.

An objective of the investigation of 2-methyl-2-nitropropane [96-jen/reu] was the state behavior of both the liquid and solid phases, including the solid−liquid phase transition. The final fit represents 18 data points (smoothed values) related to the liquid phase. No data on isothermal compressibility were available for a comparison.

The data [79-abd/dzh] for nitrobenzene at atmospheric pressure are in agreement with other values (see Apendix 1, Table 6) while large deviations from other available data were observed for the compressed-liquid region (see Table 4). The isothermal compressibilities calculated from the final fit are mostly lower than values taken from the literature (Table 5); the deviations are around 1% up to 313.15 K (including the values extrapolated toward lower temperatures and except for the value from [85-jay/red] at 313.15 K). Larger negative deviations are observed for higher temperatures.

Amides. The data available for formamide are mutually consistent, and no data points were rejected from the final fit. The deviations of calculated isothermal compressibilities from literature data are mostly positive (average deviation 4.4%) and practically the same over the temperature range from 293 to 327 K, except for $T = 298.15$ K, where the agreement is much better. A separate fit of the data [91-uos/kit] yielded $\beta_T(T = 298.15\ \text{K}, P = 0.1\ \text{MPa}) = 0.400\ \text{GPa}^{-1}$.

Except the isothermal data at $T = 298.15$ K [91-uos/kit], the analytical functions [85-eas/woo-1] were available for *N*-methylformamide. The values of volume ratio were generated from the functions (F-data, see Table 2), taking into account the solid−liquid equilibrium line [85-eas/woo-1]. The value of [91-uos/kit] at $P = 200$ MPa was rejected because of the larger positive deviation and the fact that the freezing pressure at 298.15 K is 173 MPa [85-eas/woo-1]. Fits of all three isotherms (288.15, 298.15, 313.15 K) separately resulted in the set of parameters c_0 and b_0 with a nonmonotonic temperature dependence. The final fit with $N_c = 1$ and $N_B = 2$ (see eqs 2 and 3 and Table 3) resulted

in a slightly worse description of the data compared to that of the separate isothermal fits. It is worth mentioning that the magnitude of the parameter c_1 is comparable to that of the parameter c_0.

A similar situation occurs with the data for *N*,*N*-dimethylformamide. No information on the freezing line was available. When the F-type data were generated from the functions of [85-eas/woo-1], the pressure ranges at $T = 288.15$ K and $T = 298.15$ K were, however, limited up to 100 MPa and 200 MPa, respectively, which might avoid any extrapolation to the solid-phase region (the normal melting point temperature of *N*,*N*-dimethylformamide is 213 K, i.e., 56 K lower than that of *N*-methylformamide). The final fit gives isothermal compressibilities close to the values taken from the literature; the deviations are around 1%, except for values evaluated from speed-of-sound data [76-zel/dya].

The isothermal compressibilities evaluated by Easteal and Woolf [85-eas/woo-1] for *N*-methylformamide and *N*,*N*-dimethylformamide from their smoothing functions (separate for each isotherm 288.15, 298.15, and 313.15 K) indicate that there might be a flat minimum on the temperature dependences of $\beta_T(T, P = 0.1$ MPa) around $T = 300$ K. No such behavior was observed with the fits by eq 1 (even with the separate fits for each isotherm). According to the private correspondence of the authors with Prof. L. A. Woolf, the original experimental values are not available any more and thus a detailed analysis is impossible. Therefore, new accurate experimental data are desirable to verify this unusual behavior of β_T for these two coumpounds (and possibly for formamide, as well). The scatter of β_T values calculated from speed-of-sound, volumetric, and caloric data is too large to distinguish any anomaly.

One set of isothermal data (298.15 K) was available for *N*,*N*-dimethylacetamide [91-uos/kit]. Agreement with isothermal compressibilities taken from the literature (Table 5) is good (average deviation 1.5%).

Other C−H−O−N Compounds. The fit for triethanolamine represents data of Bridgman [33-bri] for three isotherms (273.15, 323.15, and 363.15 K). No data on isothermal compressibility were available for a comparison.

The experimental temperature of measurements of 1-methoxy-2-nitrobenzene [60-hil/goc] was not found in the original source, and its value was derived by a comparison of density at atmospheric pressure with literature data (similarly for nitrobenzene). No data on isothermal compressibility were available for a comparison. It should be, however, pointed out that the data [60-hil/goc] for nitrobenzene were rejected and thus the results for 1-methoxy-2-nitrobenzene are of uncertain reliability. The low value of the parameter c_0 is rather unusual.

One set of isothermal data (298.15 K) was available for 1-methylpyrrolidin-2-one [91-uos/kit]. The deviations of isothermal compressibility calculated from the fit from values in Table 5 are negative and rather large. Both literature values of isothermal compressibility in Table 5 are derived from speed-of-sound data [94-pal/sin] and two sources of volumetric data [84-mur/rod, 89-mel/sch]. Densities at atmospheric pressure [89-mel/sch] seem to be in better agreement with single-temperature data from other sources (including [94-pal/sin]) than those of [84-mur/rod], and thus, the isothermal compressibility $\beta_T(T = 298.15$ K, $P = 0.1$ MPa$) = 0.565$ GPa^{-1} calculated using data [94-pal/sin, 89-mel/sch, 96-zab/ruz] is probably more correct.

No saturated vapor pressures or critical data were found for 3-cyanopropanal. The final fit (Table 3) was therefore performed with setting $P_{ref} = 0.101\,325$ MPa in the entire temperature range; that is, density values reported for $P = 0.1$ MPa [81-mus/gan] in the temperature range from 290.4 to 333.75 K and density values obtained by extrapolation from elevated pressures to 0.1 MPa for $T > 333.75$ K were used as the reference densities. No data for speed of sound were available, and no recommended values for isobaric heat capacity were found in [96-zab/ruz, 01-zab/ruz]. Mustafaev and Ganiev [81-mus/gan-1] published experimental isobaric heat capacities and calculated isochoric heat capacities and speeds of sound using their $P-\rho-T$ data [81-mus/gan]. The values of speed of sound calculated from eq 11 using $P-\rho-T$ data [81-mus/gan] and heat capacities [81-mus/gan-1] are, however, significantly higher than their values (e.g., in the temperature interval from 300 to 370 K and at $P = 0.1$ MPa by 10%).

C−H−O Halogen Compounds. Halogenated Alcohols. A printing error was corrected for 2-fluoroethanol [97-woo]: the density at $T = 288.15$ K and atmospheric pressure should probably be 1114.61 kg·m^{-3} instead of 1146.10 kg·m^{-3}. No data on isothermal compressibility were available for a comparison of the final fit with independent data, similarly as for 2,2-difluoroethanol.

Reasonable mutual agreement of $P-\rho-T$ data for 2,2,2-trifluoroethanol at pressures up to 40 MPa was observed. At higher pressures, the differences between [91-mal/woo] and [92-kab/yam-1] data increase up to 6 kg·m^{-3} at 200 MPa in the overlaping temperature range. Since the [91-mal/woo] data are consistent with other data in the lower temperature range, this set was retained while the [92-kab/yam-1] isotherms from 310 to 340 K were rejected. The agreement in isothermal compressibilities (Table 5) is satisfactory; the average deviation in the 10 K wide temperature interval is 1.2%. The isobaric heat capacity [96-zab/ruz] was found only for $T = 298.15$ K: $c_P = 177.8$ J·mol^{-1}·K^{-1}. This value was used to calculate isothermal compressibilities not only at 298.15 K but also at 293.15 and 303.15 K; the influence on isothermal compressibility is negligible in this case; a 1% change in heat capacity causes a 0.16% change in isothermal compressibility.

Values for 2,2,3,3,3-pentafluoropropanol and 2,2,3,3-tetrafluoropropanol were generated using the parameters of the Tait equation [94-mat/yam] separately for the temperatures 298.15 and 323.15 K. The fits in Table 3 are therefore interpolations between these two temperatures. The isothermal compressibility at $T = 298.15$ K calculated from the fit for 2,2,3,3,3-pentafluoropropanol is by about 7% lower than literature values (Table 5). A rather large discrepancy is observed for literature values of isothermal compressibility for 2,2,3,3-tetrafluoropropanol; the value calculated from the fit is between them.

The fit for 2,2,2-trichloroethanol represents the liquid-phase density data below the solid−liquid equilibrium lines for stable solid phases (denoted as s_{II}, s_I by Jenau et al. [97-jen/san]) that cross each other at the $s_{II}-s_I-l$ triple point (308.3 K, 125.6 MPa; see Figure 1). The isothermal compressibility calculated from the fit at $T = 303.15$ K is closer to the value obtained from speed of sound [98-meh/sha] and volumetric behavior [97-jen/san]. Recommended values for the isobaric heat capacity of 2,2,2-trichloroethanol were not found in [96-zab/ruz, 01-zab/ruz]; the value reported by Mehta et al. [98-meh/sha] is the value estimated by a group contribution method.

Halogenated Ethers. The data reported by Defibaugh et al. [92-gef/gil] for bis(difluoromethyl) ether cover a rather narrow pressure range (maximum pressure 5.3 MPa). The sample of purity 96.7 mol % was used for experiments (see

Table 2); the presented data are those corrected by the researchers with respect to impurity (3.3 mol % 1,1,2-trifluoroethane, HFC143). No data were available to calculate isothermal compressibility for a comparison.

Malhotra and Woolf [95-mal/woo-1] measured volume ratios $k = V(P)/V(P = 0.1\ \text{MPa})$ for two fluorinated ethers: 2,2,2-trifluoroethyl difluoromethyl ether and 1,2,2,2-tetrafluoroethyl difluoromethyl ether in a large pressure range (up to about 380 MPa). Experimental densities at atmospheric pressure are reported for the temperature ranges 274.15−293.15 K and 274.15−288.15 K, respectively. Reported volume ratios are related either to the experimental densities at $P = 0.1$ MPa (up to normal boiling point temperature) or to hypothetical values obtained by a linear extrapolation of experimental densities toward temperatures above the normal boiling point temperature (up to the highest experimental temperature 338.13 K). Densities $\rho(P)$ at each temperature were calculated from volume ratios as $\rho(P) = \rho(P = 0.1\ \text{MPa})/k$, and reference values $\rho(T,P_{\text{ref}}(T))$ for temperatures above normal boiling point temperature were obtained by extrapolation to saturation pressure using the Tait equation.

The liquid densities of pentafluoroethyl methyl ether and heptafluoropropyl methyl ether were measured in limited pressure ranges by Ohta, Widiatmo, and co-workers [01-oht/mor, 01-wid/tsu, 01-wid/uch]. The parameters of the modified BWR equation of state were evaluated by Widiatmo and Watanabe [01-wid/wat]. References to data in [01-wid/wat] are given as conference proceedings, but it is likely that the data [01-oht/mor, 01-wid/tsu, 01-wid/uch] were used. The fit presented here for heptafluoropropyl methyl ether (Table 3) represents the data in a rather limited temperature range because of instability of evaluation of parameters at temperatures close to the critical temperature. The deviations of the fits are lower than the experimental uncertainty declared by the authors (0.2%), as they are lower than 0.05%. Consequently, the weighted standard deviations are significantly lower than unity (see Table 3).

Fluorinated ethers are substances proposed as prospective refrigerants, and therefore a significant effort to measure their properties can be noticed. Besides the above-mentioned sources, there are other papers in the literature that present $P-\rho-T$ data for fluorinated ethers in the form of an equation of state. Defibaugh and Moldover [97-def/mol] evaluated parameters of the modified BWR equation of state for 16 halogenated derivatives of hydrocarbons (C_1, C_2, C_3) and two fluorinated ethers: pentafluorodimethyl ether and 2,2,2-trifluoroethyl difluoromethyl ether. Critical properties and parameters of smoothing functions for both the saturated vapor pressures and $P-\rho-T$ data are summarized in [91-wan/adc] ($CF_3OCF_2OCF_3$, $CF_3OCF_2CF_2H$, *cyclo*-$CF_2CF_2CF_2O$, CF_3OCF_2H, and CF_3OCH_3), [92-sal/wan] ($CF_3OCF_2CF_2H$, CF_3OCF_2H, CF_3OCH_3, $CF_3OCF_2OCF_3$, *cyclo*-$CF_2OCF_2OCF_2$, and *cyclo*-$CF_2CF_2CF_2O$), and [93-sal/adc] ($CF_3OCF_2CF_2CF_3$, *cyclo*-$CF_2CF_2CF_2CF_2O$, $CF_3OCF_2OCF_3$, and $CF_3OCF_2CF_2H$). A group-contribution volume-ratio method (GCVRM) to estimate the parameters of the Tait equation for fluorinated ethers was proposed by Malhotra et al. [95-mal/van].

Miscellaneous Compounds. The fits for pentafluorobenzonitrile and tetramethylstannane are correlations of values generated from the equations (the linear temperature dependence for density at 0.1 MPa and the Tait equation for the compressed-liquid region) given by Polzin and Weiss [90-pol/wei]. The deviations of the fits are therefore small and do not express the accuracy of the original experimental data. No data on isothermal compressibility were found for pentafluorobenzonitrile for a comparison. The isothermal compressibilities for tetramethylstannane in the temperature range from 293.15 to 303.15 K are compared in Table 5. Values calculated from the fit are mostly lower (average deviation 2.5%) than values based on speed-of-sound data [80-keh/vog]. A positive deviation is observed for the value reported by Delmas et al. [78-phi/del, 84-rie/del] at 298.15 K calculated from isobaric thermal expansivity and thermal pressure coefficients, $\beta_T = \alpha_P/\gamma_V$. The coefficient of isobaric expansivity given by Delmas et al. (1.28 kK^{-1}) is, however, significantly lower than values from the fits of densities (1.380 kK^{-1} [77-ahm/dix] and 1.385 kK^{-1} [90-pol/wei]).

The data available for tetramethylsilane are not in mutual agreement. Separate fits of the data at $T = 298.15$ K yielded $\beta_T(T = 298.15\ \text{K}, P = 0.1\ \text{MPa}) = 2.519\ \text{GPa}^{-1}$ [75-par/jon], 2.677 GPa^{-1} [89-bao/cac], and 2.927 GPa^{-1} [90-yok/tak]. The final fit is based on data in the low temperature range [89-bao/cac], in the middle temperature range [90-yok/tak], and at high temperatures [75-par/jon]. The deviations from isothermal compressibilities taken from the literature are therefore negative at low temperatures and become positive at temperatures close to 298.15 K (Table 5). The isothermal compressibilities reported by McLure et al. [94-mcl/bar] were obtained from speed-of-sound data in the temperature interval from 224.86 to 273.28 K using the same values of isobaric heat capacity as those recommended in [96-zab/ruz]; the densities and isobaric thermal expansivities reported in [94-mcl/bar] are slightly higher (by 0.2% and 4%, respectively) than those resulting from density data [89-bao/cac].

The fits for tetraethylsilane and tetraethoxysilane represent the data measured by Yokoyama et al. [90-yok/tak]. Agreement with isothermal compressibilities (Table 5) is very satsifactory (average deviations 2.1% and 1.8%, respectively). It should be pointed out that the heat capacity values for tetraethylsilane in the temperature range from 303.15 to 333.15 K were obtained by a quasi-polynomial extrapolation [96-zab/ruz] from experimental data at lower temperatures. The deviations of the isothermal compressibilities of tetraethoxysilane are positive except for the value from [78-phi/del] that was obtained from isobaric expansivity and thermal pressure coefficients, $\beta_T = \alpha_P/\gamma_V$. The coefficient of isobaric thermal expansivity reported in [78-phi/del] (1.168 kK^{-1}) is, however, slightly higher than that evaluated from density data (1.123 kK^{-1}) [90-yok/tak].

The data reported for hexamethyldisilane by Briese and Wuerflinger [82-bri/wue] cover mostly the solid-phase region. After the value at 313.2 K and 30 MPa was rejected (too high density, probably because of partial solidification of the sample), seven liquid-density data points remained for the final fit that represents data along three isotherms (303.2, 313.2, and 323.2 K).

The data available for octamethylcyclotetrasiloxane are not in mutual agreement. The data at $T = 323.15$ K from [84-eas/woo] are lower than values from an extensive set [76-ben/win] (deviations up to 4.5 $\text{kg}\cdot\text{m}^{-3}$), and a separate fit yielded $\beta_T(T = 323.15\ \text{K}, P = 0.1\ \text{MPa}) = 1.572\ \text{GPa}^{-1}$, which is too low (Table 5). The isothermal compressibilities calculated from a separate fit of data from [96-wap/tar] are, on the other hand, higher (e.g., $\beta_T(T = 308.80\ \text{K}, P = 0.1\ \text{MPa}) = 1.716\ \text{GPa}^{-1}$). The final fit represents data by Benson and Winnick [76-ben/win]; the agreement in isothermal compressibilities is satisfactory (Table 5), even for values extrapolated more than 20 K beyond the tempera-

ture range of the fit. There are, however, large negative deviations when the isothermal compressibilities calculated from the fit are compared with values obtained from speed-of-sound, volumetric, and heat capacity data. Two sources of data for speed of sound [58-wat/van, 80-nie/sch] report nearly identical values at 293.15 K (933.1 and 935.3 $m \cdot s^{-1}$). The volumetric data (ρ and α_P) used seem to be correct, since the isothermal compressibilities obtained from values of the thermal pressure coefficient [63-ros/hil] and independent evaluations of α_P are within 2% identical with those reported in the same source [63-ros/hil]. Isobaric heat capacities [96-zab/ruz] are based on measurements by Mekhtiev et al. [75-mek/kar] (e.g., $c_P(T = 298.15\ K) = 337.9\ J \cdot mol^{-1} \cdot K^{-1}$). If the value of c_P in eq 11 is varied (using speed-of- sound data [80-nie/sch]), then with $c_P(T = 298.15\ K) = 469\ J \cdot mol^{-1} \cdot K^{-1}$ the value identical with that measured directly (using a dilution piezometer) by Ewing and Marsh [77-ewi/mar] ($\beta_T(T = 298.15\ K) = 1.531\ GPa^{-1}$) can be obtained. This indicates that the heat capacity data [75-mek/kar] might be lower than correct values. The approximate value of the heat capacity of octamethylcyclotetrasiloxane ($c_P(T = 291.15\ K) \approx 500\ J \cdot mol^{-1} \cdot K^{-1}$) derived from a comparison with the rate of cooling of glacial acetic acid [53-ost/gru] supports the above conclusion.

Density values for the fit for dimethyl sulfoxide were generated from equations reported in [80-fuc/ghe] in the form of a quadratic function of pressure, the parameters of which are given separately for each of four temperatures in the range from 293.6 to 323.0 K. The fit with $N_B = 1$ (eq 3) only was selected, since an extreme appeared on the $B(T)$ dependence at $T = 319$ K with $N_B = 2$. The extreme $B(T)$ corresponds to the extreme on the $\beta_T(T)$ dependence, but here the existence of this anomalous behavior should be verified using more data (preferably direct experimental ones). The agreement for the isothermal compressibilities (Table 5) is good for temperatures up to 303 K; at higher temperature, larger negative deviations are observed.

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Appendix 1

Representation of Reference Density Data $\rho[T,P_{ref}(T)] = \rho(T)$**.** The functions of temperature selected to represent reference density data $\rho[T, P_{ref} = 0.101\ 325\ MPa$ or $P_{ref} = P_{sat}(T)] = \rho(T)$ are as follows

$$\rho(T/K)/(kg \cdot m^{-3}) = \rho_c\{1 + \sum_{i=0}^{5} a_i(1 - T_r)^{(i+1)/3}\}, \quad T_r = T/T_c \quad (12)$$

$$\rho(T/K)/(kg \cdot m^{-3}) = \sum_{i=0}^{4} a_i(T/100)^i \quad (13)$$

The values of the adjustable parameters a_i obtained by fitting to selected data using a weighted least-squares method are recorded in Table 6 along with some characteristics of the fits. The statistical weights of density values were estimated from information in the original papers. The absence of extremes and inflection points on the function $\rho(T)$ was checked for all fits. Equation 12 was preferably used in those cases where respective critical parameters (ρ_c, T_c) were available to enlarge the use of the fits beyond the temperature range of the data, particularly in the region between T_{max} and T_c. Therefore, the fits by eq 12 with $a_0 > 0$ were selected to get the correct derivative of the liquid−vapor saturation line at the critical point, $(d\rho/dT) \rightarrow -\infty$ for $T \rightarrow T_c$.

The fits of selected data on reference densities are presented here as auxiliary information that might be useful, particularly for less common substances. Any other data at the reference pressure may be, however, employed for the practical use of the fits given in Table 3 to calculate densities at elevated pressures, for example, the densities of a particular liquid sample, data taken from critical evaluations, and so forth. The fits in Table 3 are independent of the data given in Table 6 in those cases where either original reference densities or values obtained by extrapolation from particular compressed-liquid density data (denoted as "o" or "p" in Table 4, respectively) were used for the fits. Reference density values calculated from smoothing functions (Table 6) were employed for some data sets (RD = "e", Table 4) for ethanenitrile, 2,2,2-trifluoroethanol, bis(difluoromethyl) ether, and pentafluoroethyl methyl ether.

The results in Table 6 are either (i) the fits of recommended values available in the literature [86-trc, 90-cha/gad, 93-das/fre] or (ii) the fits of reference densities presented by the authors of respective data at elevated pressures or (iii) the fits employed for evaluation of isothermal compressibilities (Table 5) or (iv) the fits of data taken from selected sources that present results of measurements at atmospheric or saturation pressure in wider temperature ranges. In a few cases, the density reported by the authors of isothermal $P-\rho-T$ data at one temperature is recorded in Table 6 ($T_{min} = T_{max}$ and $\rho = a_0$ (eq 13) hold in these cases). With the exception of fits i, the other fits in Table 6 are not the results of a critical evaluation; that is, not all available data were considered. No parameters are presented for those substances where the compressed-liquid $P-\rho-T$ data were reported in the original sources as relative properties (relative density, volume ratio, compression), and no densities at reference pressure were needed for other purposes (1,2-ethanediamine, 2-methylpropanenitrile, phenylethanenitrile, triethanolamine). A few remarks concerning the fits are given below.

Data [79-gus/far] for 2-methyl-1-aminobenzene up to the normal boiling point (473.5 K) are lower by 2.9 $kg \cdot m^{-3}$ (average deviation) than those represented by the fit of the data [90-cha/gad]. The deviations between the densities for 4-methyl-1-aminobenzene [81-gus/naz, 90-cha/gad] are of the same sign but, however, are much larger (e.g., −10 $kg \cdot m^{-3}$ at 323 K, −155 $kg \cdot m^{-3}$ at 448 K) and difficult to explain.

The fit for acetonitrile is predominantly based on values obtained by Kratzke and Mueller [85-kra/mue] by an extrapolation of their compressed-liquid data. The temperature range of the fit is enlarged by retaining rather inaccurate data [75-fra/fra] (the uncertainty declared by the researchers is 1 $kg \cdot m^{-3}$). A comparison of the fit with selected data from other sources in the range from 278.15 to 348.16 showed deviations within 0.4 $kg \cdot m^{-3}$. No experimental data were available for ethanenitrile-d_3; the fit in Table 6 represents an interpolation of values obtained by extrapolation of compressed-liquid density data to atmospheric pressure (three isotherms).

The inflection point appears on function 12 for benzonitrile at $T = 364$ K. Density values at $T > 473$ K were obtained by the extrapolation of rather imprecise compressed-liquid densities (see RMSD = 1.858 $kg \cdot m^{-3}$ of the [78-gus/naz] data in Table 4) to saturated vapor pressure.

Their reliability is doubtful, and retaining them may cause a distortion of the fit.

The two fits that are presented for 1-methylpyrrolidin-2-one differ from each other by 3.2 kg·m^{-3} (0.3%) in the overlaping temperature range from 283.15 to 298.15 K. The fit of the [89-mel/sch] data gives higher densities and isobaric thermal expansivities (by 5.6% on average) than those of the [84-mur/rod] data. The effect of this discrepancy on the isothermal compressibility calculated using eq 11 is significant (see Table 5).

As was mentioned above, a printing error was corrected for 2-fluoroethanol. The density value reported for T = 288.15 K (1146.10 kg·m^{-3}) was replaced by the value which is probably correct (1114.61 kg·m^{-3}) and lies close to the smooth curve obtained using data for other temperatures. Two fits each are presented for 2,2,3,3,3-pentafluoropanol and 2,2,3,3-tetrafluoropanol. The first one represents experimental data [96-nak/sak]; the second one is a linear interpolation of values [94-mat/yam]. Densities [96-nak/sak] are lower for both alcohols. Differences between the fits are, on average, 1.3 kg·m^{-3} (2,2,3,3,3-pentafluoropanol) and 2.5 kg·m^{-3} (2,2,3,3-tetrafluoropanol) in the overlaping temperature range.

Experimental densities [95-mal/woo-1] for 2,2,2-trifluoroethyl methyl ether and 1,2,2,2-tetrafluoroethyl methyl ether were available in the temperature ranges 274.15−293.15 K and 274.15−288.15 K, respectively. Densities at higher temperatures (above the normal boiling point temperatures up to 338.15 K) were obtained by extrapolation using the modified Rackett equation [85-cam/tho]. The average deviation between the fitted set of both the experimental and extrapolated values [95-mal/woo-1] and the function [97-def/mol] for 2,2,2-trifluoroethyl methyl ether (see Table 6) is 0.44 kg·m^{-3}, which confirms a good performance of the extrapolations for the two ethers. Also, the agreement of critical densities obtained from the extrapolation with the values from other sources is very good: 506 kg·m^{-3} for 2,2,2-trifluoroethyl methyl ether (the estimated value reported in [97-def/mol] is 515.6; that is, the deviation is 1.9%) and 556 kg·m^{-3} for 1,2,2,2-tetrafluoroethyl methyl ether (the experimental value [96-sak/sat] is 533 kg·m^{-3}; that is, the deviation is 4.2%).

The fits for pentafluorobenzonitrile and tetramethylstannane are recorrelations of the values generated from the linear functions $\rho(T)$ given by Polzin and Weiss [90-pol/wei]. The densities of tetramethylstannane taken from other source [77-ahm/dix] are, however, significantly lower (deviations are between 19.2 and 21.6 kg·m^{-3} in the overlaping temperature range), but the values of thermal expansivity α_P differ by about 1% only.

Two fits are presented for octamethylcyclotetrasiloxane. The first fit, which is valid for a slightly wider temperature range, gives higher densities than the second one; the average deviation between the fits is 0.39 kg·m^{-3}.

The first fit given in Table 6 for dimethyl sulfoxide represents values calculated from polynomial functions of pressure given for each of four experimental temperatures in [80-fuc/ghe]. The second fit represents experimental data taken from 22 various sources (not cited here); the value of RMSD = 0.16 kg·m^{-3} indicates good agreement between the data. Densities calculated from the first fit are significantly higher (deviations 1.8 kg·m^{-3} at 296.6 K, 4.3 kg·m^{-3} at 323.0 K; average deviation 3.1 kg·m^{-3}).

Appendix 2

Parameters of the Wagner Function for Saturated Vapor Pressure. Saturated vapor functions for several substances were not found in the literature or in the database [93-cda], or the form of the function was different from that of eq 14 below. The available data for those substances were correlated by the Wagner function

$$\ln(P_s/P_c) = \{a_0(1 - T_r) + a_1(1 - T_r)^{1.5} + a_2(1 - T_r)^{2.5} + a_3(1 - T_r)^5\}/T_r \qquad T_r = T/T_c \quad (14)$$

where P_s is the saturated vapor pressure and P_c and T_c are the critical pressure and the critical temperature, respectively. The adjustable parameters of eq 14, the critical properties, and references to literature sources of data are given in Table 7. The temperature ranges T_{min}, T_{max} are the ranges of data for $T < T_c$ used to evaluate the parameters. The temperature ranges cover a wide interval from the normal boiling point temperature (or lower temperature) up to the critical temperature, except for 2-methylpropenenitrile, for which the Antoine equation was used to obtain the saturation pressure slightly above the normal boiling point temperature needed for the correlation of $P-\rho-T$ data.

Experimental data for 1,2,2,2-tetrafluoroethyl difluoromethyl ether were not found in the literature. Susay et al. [96-sus/smi] reported parameters of the Antoine equation of desflurane (according to our knowledge, the names (−)-desflurane and (+)-desflurane are used for optical isomers of 1,2,2,2-tetrafluoroethyl difluoromethyl ether, employed as an anaesthetic agent) valid in the temperature range from 274.15 to 311.25 K. The normal boiling point temperature issuing from their equation (295.5 K) is by 1 K lower than that reported in [98-mat/tan]. Since the accuracy of these data is rather uncertain and the temperature range is limited, saturated vapor pressures were estimated using the Riedel method [54-rie] and then fitted by eq 14.

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