Reviews

$P-\rho-T$ Data of Liquids: Summarization and Evaluation. 7. Selected Halogenated Hydrocarbons

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The published experimental data for 41 halogen derivatives of hydrocarbons (2 fluoro derivatives, 22 chloro derivatives, 11 bromo derivatives, and 6 iodo derivatives) are summarized and reviewed, and the parameters of the Tait equation are given for 39 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 density 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 a continuation of a systematic summarization and critical evaluation of published $P-\rho-T$ 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] and C−H−O substances [94-cib/zik, 97-cib/hne, 97-cib/hne-1] have already been reviewed and evaluated. This work concerns the group of selected halogenated (F, Cl, Br, I) hydrocarbons for which the available published experimental values of density, $\rho(T,P)$, relative density, $\rho(T,P)/\rho(T,P = 0.1$ MPa or $P_{sat})$, and related quantities of liquids were compiled from the literature and evaluated. Fluorinated (except for derivatives of benzene) and mixed-halogenated hydrocarbon derivatives, that involve mainly industrially important substances used as refrigerants or heat-pump fluids, were omitted from the present work since there are already comprehensive publications on thermodynamic properties of pure refrigerants (including $P-\rho-T$ behavior) available in the open literature. Among them the following selected reviews may be mentioned: trichlorofluoromethane (R-11) [92-jac/pen], dichlorodifluoromethane (R-12) [92-pen/jac], chlorodifluoromethane (R-22) [92-kam/bey], difluoromethane (R-32) [95-out/mcl, 97-til/yok], 1,1,1-trifluoro-2,2-dichloroethane (R-123) [94-you/mcl], pentafluoroethane (R-125) [95-out/mcl, 98-pia/nog, 98-sun/til], 1,1,1,2-tetrafluoroethane (R-134a) [94-til/bae], 1,1,1-trifluoroethane (R-143a) [97-out/mcl, 98-pia/fuj, 99-li /til], 1,1-difluoroethane (R-152a) [96-out/mcl]. JAR Tables [94-jar] summarize properties for 12 refrigerants (R-23, 32, 123, 124, 125, 134a, 141b, 142b, 143a, 152a, 225ca, 225cb); constants of the Tait equation for nine refrigerants (R-11, 12, 22, 32, 124, 125, 134a, 141b, 152a) are reported by Assael et al. [95-ass/dym]; correlation and prediction methods may be found in papers [93-mal/woo, 98-dym]; a literature survey for refrigerant blends (R-404A, 407C, 410A) was presented by Krauss and Stephan [98-kra/ste]. The electronic database REFPROP developed at NIST [98-mcl/kle] provides calculated values of thermodynamic and transport properties for 26 pure refrigerants (along with ammonia, carbon dioxide, ethane, propane, propene, butane, and 2-methylpropane) and their 31 predefined mixtures.

Sources of Data

The original experimental data (5250 data points for 41 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 (CASRN) 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 taken 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−h in Table 2). Similarly, as in our previous reviews, values (denoted by the 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

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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

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

where

$$C(T,\vec{c}) = \sum_{i=0}^{N_{\mathrm{C}}} c_i[(T - T_0)/100]^i$$

$$\vec{c} = \{c_i\} = \{c_0, ..., c_{N_{\mathrm{C}}}\} \quad (2)$$

$$B(T,\vec{b}) = \sum_{i=0}^{N_{\mathrm{B}}} b_i[(T - T_0)/100]^i$$

$$\vec{b} = \{b_i\} = \{b_0, ..., b_{N_{\mathrm{B}}}\} \quad (3)$$

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, $\rho(T,P_{\mathrm{ref}}(T))$ and $P_{\mathrm{ref}}(T)$, were selected in the same way as that used previously; that is, at temperatures below the normal boiling temperature the densities at atmospheric pressure ($P_{\mathrm{ref}} = 0.101\,325$ MPa) were used, while for higher temperatures the values along the saturation curve, that is, saturated liquid densities and saturated vapor pressures, were employed. 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, $\rho(T,P_{\mathrm{ref}})$, and thus the values of relative density, $\rho(T,P)/\rho(T,P_{\mathrm{ref}} = 0.1$ MPa or $P_{\mathrm{sat}})$, reported by the authors were correlated by eq 1. In some cases of isothermal data the reference density, $\rho(T,P_{\mathrm{ref}})$, was obtained for each isotherm by an extrapolation of experimental compressed-liquid density data to reference pressure, P_{ref} (0.101 325 MPa below or P_{sat} above 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 7) 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, $\rho(T,P)/\rho(T,P_{\mathrm{ref}})$; volume ratio, $V(T,P)/V(T,P_{\mathrm{ref}}) = \rho(T,P_{\mathrm{ref}})/\rho(T,P)$; compression, $\{V(T,P_{\mathrm{ref}}) - V(T,P)\}/V(T,P_{\mathrm{ref}}) = 1 - \rho(T,P_{\mathrm{ref}})/\rho(T,P)$), such data were correlated by eq 1 without any knowledge of reference densities; that is, the relative densities $\rho(T,P)/\rho(T,P_{\mathrm{ref}})$ were correlated.

Saturated vapor pressures were calculated from the smoothing functions taken from the literature (for references, see Table 3) and used in the correlations. For several substances the Wagner function was obtained from experimental data in limited temperature ranges (see Appendix 2), and thus the values interpolated between the value corresponding to the highest experimental temperature and critical pressure were used in the correlations.

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
Methane Derivatives		
chloromethane	74-87-3	CH_3Cl
dichloromethane	75-09-2	CH_2Cl_2
trichloromethane (chloroform)	67-66-3	$CHCl_3$
tetrachloromethane	56-23-5	CCl_4
bromomethane	74-83-9	CH_3Br
dibromomethane	74-95-3	CH_2Br_2
tribromomethane (bromoform)	75-25-2	$CHBr_3$
iodomethane	74-88-4	CH_3I
diiodomethane	75-11-6	CH_2I_2
Ethane and Ethene Derivatives		
chloroethane	75-00-3	C_2H_5Cl
1,1-dichloroethane	75-34-3	$C_2H_4Cl_2$
1,2-dichloroethane	107-06-2	$C_2H_4Cl_2$
1,1,1-trichloroethane	71-55-6	$C_2H_3Cl_3$
1,1,2-trichloroethane	79-00-5	$C_2H_3Cl_3$
1,1,2,2-tetrachloroethane	79-34-5	$C_2H_2Cl_4$
chloroethene	75-01-4	C_2H_3Cl
cis-1,2-dichloroethene	156-59-2	$C_2H_2Cl_2$
trans-1,2-dichloroethene	156-60-5	$C_2H_2Cl_2$
trichloroethene	79-01-6	C_2HCl_3
tetrachloroethene	127-18-4	C_2Cl_4
bromoethane	74-96-4	C_2H_5Br
1,2-dibromoethane	106-93-4	$C_2H_4Br_2$
Propane Derivatives		
1-chloropropane	540-54-5	C_3H_7Cl
1-bromopropane	106-94-5	C_3H_7Br
2-bromopropane	75-26-3	C_3H_7Br
1-iodopropane	107-08-4	C_3H_7I
Butane Derivatives		
1-chlorobutane	109-69-3	C_4H_9Cl
1-bromobutane	109-65-9	C_4H_9Br
1-iodobutane	542-69-8	C_4H_9I
Pentane Derivatives		
1-chloropentane	543-59-9	$C_5H_{11}Cl$
1-bromopentane	110-53-2	$C_5H_{11}Br$
1-iodopentane	628-17-1	$C_5H_{11}I$
Derivatives of Cyclic Hydrocarbons		
fluorobenzene	462-06-6	C_6H_5F
hexafluorobenzene (perfluorobenzene)	392-56-3	C_6F_6
chlorobenzene	108-90-7	C_6H_5Cl
1,2-dichlorobenzene	95-50-1	$C_6H_4Cl_2$
chlorocyclohexane	542-18-7	$C_6H_{11}Cl$
2,4-dichloro-1-methylbenzene (2,4-dichlorotoluene)	95-73-8	$C_7H_6Cl_2$
bromobenzene	108-86-1	C_6H_5Br
2,4-dibromo-1-methylbenzene (2,4-dibromotoluene)	31543-75-6	$C_7H_6Br_2$
iodobenzene	591-50-4	C_6H_5I

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

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

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

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]	date type[b]	sample purity[c] / %
Chloromethane								
64-hsu/mck	169	308.15	413.15	0.8	31.6	vl	D[f]	>99.9[e]
78-kum/iwa	32	253.15	313.15	28.7	159.5	vl	D	99.5[d]
total	201	253.15	413.15	0.8	159.5			
Dichloromethane								
49-bri	11	298.15	298.15	49.0	980.7	vs	D	
51-new/wea	5	298.15	298.15	40.5	101.3	va	D	
65-sch/has	8	298.15	298.15	20.0	90.0	vs	F	
70-sch/eck	18	303.15	323.15	18.0	518.9	vb	D	
75-bur/ric	20	293.15	298.15	1.0	10.0	ce	F	99.88m[d]
81-dic	17	295.00	295.00	650.0	51100.0	sw	D	
82-kum/tak	21	298.15	348.15	10.1	101.3	nd	D	
85-dig/deu	77	303.20	423.20	1.0	200.0	pe	D	
85-eas/woo	3	298.15	298.15	5.0	100.0	vb	S	
91-bao/cac	25	298.15	298.15	0.6	102.0	rl	D[g]	99.5m[d]
total	205	293.15	423.20	0.6	51100.0			
Trichloromethane								
49-bri	10	298.15	298.15	49.0	490.3	vs	D	
51-new/wea	1	298.15	298.15	101.3	101.3	va	D	
51-new/wea	6	298.15	298.15	40.5	101.3	va	D	
72-lys	2	297.15	297.15	327.0	623.0	sw	D	
75-bur/ric	20	293.15	298.15	1.0	10.0	ce	F	>99m[d]
81-dic	20	295.00	295.00	2700.0	60900.0	sw	D	
82-kum/tak	28	273.15	348.15	10.8	98.7	nd	D	99.55w[e]
84-eas/woo	5	298.15	298.15	50.0	250.0	vb	D	98.5[e]
85-eas/woo	3	298.15	298.15	25.0	100.0	vb	S	98[d]
87-nhu/bha	5	293.15	293.15	2.0	10.0	mo	D	99.95[e]
total	100	273.15	348.15	1.0	60900.0			
Tetrachloromethane								
31-bri	10	323.15	368.15	49.1	343.3	vb	D	
41-gib/loe	20	298.15	338.15	25.0	100.0	vl	F	
57-wal/ric	2	295.15	298.15	7390.0	17100.0	sw	D	
62-hol/wha	50	298.15	348.15	1.0	10.0	vl	F	>99.9[e]
65-sch/has	8	298.15	298.15	20.0	90.0	vs	F	
69-mop	22	273.15	323.15	10.2	197.7	vb	D	
70-dic	35	295.00	295.00	2700.0	63300.0	sw	D	>99[d]
73-rog/bur	10	298.15	298.15	1.0	10.0	ce	F	
75-bur/ric	20	293.15	298.15	1.0	10.0	ce	F	
76-ben/win	463	273.15	413.17	0.4	338.0	vb	D[h]	99.99[e]
78-han/gup	24	273.15	363.15	2.8	22.1	cs	D	
86-eas/woo	64	308.15	338.15	1.1	250.2	vb	D	
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[h]	>99.8m[e]
87-lai/mil	123	329.81	408.81	0.2	55.7	hp	S[h]	99.97w[d]
total	856	273.15	413.17	0.2	63300.0			
Bromomethane								
78-kum/iwa	32	253.15	313.15	28.7	159.5	vl	D	99.8[d]
88-rut	8	293.15	363.15	0.8	7.0	rl	D	99.5[d]
total	40	253.15	363.15	0.8	159.5			
Dibromomethane								
81-dic	11	295.00	295.00	4390.0	70000.0	sw	D	
Tribromomethane								
31-bri	10	323.15	368.15	49.1	343.3	vb	D	
Iodomethane								
78-kum/iwa	32	253.15	313.15	28.7	159.5	vl	D	98.2[d]
Diiodomethane								
72-lys	2	297.15	297.15	692.0	1536.0	sw	D	
81-dic	11	295.00	295.00	2190.0	81700.0	sw	D	
total	13	295.00	297.15	692.0	81700.0			
Chloroethane								
88-rut	12	293.15	423.15	0.3	5.0	rl	D	99.7[d]
1,1-Dichloroethane								
51-new/wea	7	298.15	298.15	40.5	101.3	va	D	>98.0m[d]
85-kum/tak	35	298.15	398.15	10.1	101.3	vs		
total	42	298.15	398.15	10.1	101.3			
1,2-Dichloroethane								
51-new/wea	6	298.15	298.15	40.5	101.3	va	D	
85-kum/tak	35	298.15	398.15	10.1	101.3	vs	D	>99.9m[d]
90-mal/pri	125	278.15	338.15	2.5	280.0	vb	F	99.0m[d]
94-mal/woo	117	278.15	338.15	2.5	394.4	vb	D[h]	>99.0[d]
96-hah/ulc	5	293.15	293.15	2.0	10.0	mo	D	99.999m[e]
total	288	278.15	398.15	2.0	394.4			
1,1,1-Trichloroethane								
89-kum	35	298.15	398.15	10.1	101.3	vs	D	95.9w[e]
1,1,2-Trichloroethane								
89-kum	35	298.15	398.15	10.1	101.3	vs	D	99.6w[e]
1,1,2,2-Tetrachloroethane								
51-new/wea	6	298.15	298.15	40.5	101.3	va	D	
63-and	8	295.25	295.25	142.3	459.2	va	D	
total	14	295.25	298.15	40.5	459.2			
Chloroethene								
82-cul/ely	69	280.99	337.25	0.4	4.1	mo	D	99.995[e]
***cis*−1,2-Dichloroethene**								
96-hah/ulc	5	293.15	293.15	2.0	10.0	mo	D	99.2m[e]
***trans*−1,2-Dichloroethene**								
51-new/wea	7	298.15	298.15	40.5	101.3	va	D	
96-hah/ulc	5	293.15	293.15	2.0	10.0	mo	D	99.4m[e]
total	12	293.15	298.15	2.0	101.3			
Trichloroethene								
51-new/wea	6	298.15	298.15	40.5	101.3	va	D	
Tetrachloroethene								
51-new/wea	7	298.15	298.15	40.5	101.3	va	D	
Bromoethane								
42-bri	8	298.15	348.15	980.7	2794.9	vs	D	
57-wal/ric	2	289.15	292.15	6800.0	15710.0	sw	D	
69-mil/jen	70	203.15	298.15	24.5	588.4	nd	D	99.6[e]
78-kum/iwa	32	253.15	313.15	19.7	156.8	vl	D	99[d]
88-rut	10	293.15	393.15	0.3	5.0	rl	D	99.99[e]
total	122	203.15	393.15	0.3	15710.0			
1,2-Dibromoethane								
60-hil/goc	5	293.15	293.15	6.1	42.6	bu	D	
68-ski/cus	2	303.15	303.15	53.4	71.2	vm	D	
total	7	293.15	303.15	6.1	71.2			
1-Chloropropane								
33-bri	41	273.15	368.15	49.0	1176.8	vb	D	
88-rut	12	293.15	423.15	0.3	5.0	rl	D	99.6[e]
total	53	273.15	423.15	0.3	1176.8			
1-Bromopropane								
33-bri	42	273.15	368.15	49.0	1176.8	vb	D	
42-bri	6	298.15	348.15	980.7	2020.2	vs	D	
71-jen/mil	84	203.15	323.15	24.5	588.4	nd	D	98.7[e]
78-gus/bai	131	280.00	500.00	5.0	100.0	bu	D	99.98w[e]
88-rut	10	293.15	393.15	0.3	5.0	rl	D	99.6[e]
total	273	203.15	500.00	0.3	2020.2			
2-Bromopropane								
78-gus/bai	110	280.00	450.00	5.0	100.0	bu	D	99.97w[e]
1-Iodopropane								
33-bri	41	273.15	368.15	49.0	1176.8	vb	D	
1-Chlorobutane								
33-bri	41	273.15	368.15	49.0	1176.8	vb	D	
68-ski/cus	5	303.15	303.15	101.3	486.4	vl	D	
88-rut	12	293.15	423.15	0.3	5.0	rl	D	
total	58	273.15	423.15	0.3	1176.8			
1-Bromobutane								
33-bri	42	273.15	368.15	49.0	1176.8	vb	D	
42-bri	18	298.15	348.15	980.7	4903.3	vs	D	
69-mil/jen	111	203.15	373.15	24.5	588.4	nd	D	99.99[e]
total	171	203.15	373.15	24.5	4903.3			
1-Iodobutane								
33-bri	42	273.15	368.15	49.0	1176.8	vb	D	
1-Chloropentane								
33-bri	40	273.15	368.15	49.0	1176.8	vb	D	
1-Bromopentane								
33-bri	38	273.15	368.15	49.0	1176.8	vb	D	
71-jen/mil	97	248.15	398.15	24.5	588.4	nd	D	99.0[e]
77-gus/bai	143	283.00	523.00	5.0	98.1	bu	D	99.8[e]
total	278	248.15	523.00	5.0	1176.8			
1-Iodopentane								
33-bri	41	273.15	368.15	49.0	1176.8	vb	D	
Fluorobenzene								
74-de /fin[i]	41	303.15	523.15	6.0	350.0	vb	D	>99[e]
89-abd/akh	80	298.15	548.15	2.4	50.6	pi	D	99.96w[e]
91-ver/mel	121	293.00	423.00	10.0	600.0	vb	D	
total	242	293.00	548.15	2.4	600.0			
Hexafluorobenzene								
80-hog/kri	34	288.15	423.15	20.0	250.0	vb	S	98.7[e]
81-dym/rob	23	298.21	373.18	19.2	303.5	nd	S	
82-dym/gle	6	298.11	373.10	0.4	36.3	mo	D	99m[d]
82-dym/gle	13	298.11	373.10	53.5	310.4	vb	D	99m[d]
total	76	288.15	423.15	0.4	310.4			

Table 2. (Continued)

ref	N_p	T_{min} K	T_{max} K	P_{min} MPa	P_{max} MPa	meth[a]	date type[b]	sample purity[c] %
Chlorobenzene								
31-bri	28	273.15	368.15	49.1	1078.8	vb	D	
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	
42-bri	2	348.15	348.15	980.7	1274.9	vs	D	
49-bri	10	298.15	298.15	49.0	490.3	vs	D	
63-and	2	298.15	298.15	262.2	452.1	va	S	
68-ski/cus	10	303.15	303.15	35.7	498.5	vl	D	
70-sch/eck	9	303.15	323.15	46.7	509.6	vb	D	
73-aga/kaf	108	308.25	583.15	0.2	32.5	hp	D	99.6[e]
75-gus/mir	66	293.00	579.35	5.0	50.1	bu	D	99.5[e]
76-aga/kaf	288	303.15	632.15	0.3	41.9	pi	D	99.96w[e]
80-tak	4	298.15	298.15	55.3	206.9	ul	C	>99.0v[e]
82-tak/ter	20	303.15	303.15	10.0	200.0	ul	C	
83-kas/fuk	40	298.15	398.15	0.2	98.2	cl	D	99.0m[d]
84-abd/dzh	117	298.15	623.15	1.3	50.0	pi	D	99.90w[e]
90-won/hay	18	298.20	348.20	0.7	6.9	mo	D	99.9[d]
91-ver/mel	132	293.00	423.00	10.0	600.0	vb	D	
97-eas/bac	138	278.15	338.13	1.9	283.1	vb	D[g]	99.5[d]
total	1014	273.15	632.15	0.2	1274.9			
1,2-Dichlorobenzene								
97-eas/bac	115	278.15	338.13	2.5	311.5	vb	D[g]	>99[d]
Chlorocyclohexane								
97-jen/wue	109	228.15	298.15	10.0	280.0	vs	S	99.5[e]
2,4-Dichloro-1-methylbenzene								
91-ver/mel	106	293.00	423.00	10.0	600.0	vb	D	
Bromobenzene								
31-bri	20	273.15	368.15	49.1	882.7	vb	D	
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	
82-tak/ter	20	303.15	303.15	10.0	200.0	ul	C	
87-eas/woo	66	278.15	323.15	2.5	280.0	vb	F	
total	128	273.15	368.15	2.5	882.7			
2,4-Dibromo-1-methylbenzene								
91-ver/mel	111	293.00	423.00	10.0	600.0	vb	D	
Iodobenzene								
91-ver/mel	120	293.00	423.00	10.0	600.0	vb	D	

[a] Method used for measurements: bu, buoyancy method; ce, densities evaluated by integration from isothermal compressibilities obtained by ultracentrifuge method; cl, constant volume cell with liquid piston; cs, constant volume cell with solid piston; hp, high-pressure pycnometer; mo, mechanical oscillator method; nd, not described or stated in the reference; pe, permittivity method; pi, piezometer of unspecified type; rl, expansion principle; sw, shock wave method; ul, densities evaluated from speeds of sound; va, Aime method; vb, variable-volume cell with bellows; vl, variable-volume cell with liquid piston; 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, 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-48 declared by the researchers. [g] ITS-90 declared by the researchers. [h] IPTS-68 declared by the researchers. [i] Density data for C_6H_5F (not for C_6D_5F).

4, were defined as

$$w_j = \mu_j/(\delta\rho_j)^2 \tag{5}$$

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 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 dibromomethane and diiodomethane, since the only experimental data found in the literature were those obtained by the shock-wave method at extremely high pressures. Isothermal compressibilities at atmospheric pressure calculated from tentative fits differed by several hundreds of a percent from values compiled from the literature, and thus an interpolation between atmospheric pressure and those of data using eq 1 would be highly unreliable.

Table 3 records the values of the parameters of eq 1 for 39 substances along with some statistical information of the fits defined as follows:

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

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

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

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

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

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 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.

Temperature and pressure ranges of validity of the fits given in the table allow one to avoid extrapolation using

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, and References to Saturated Vapor Pressure, ref(P_{sat}), for the Fits Where T_{Max} Is Higher Than the Normal Boiling Temperature

	chloromethane	dichloromethane	trichloromethane	tetrachloromethane
c_0	0.098986	0.097637	0.095721	0.093334
b_0/MPa	30.0681	94.5164	92.1638	27.9102
b_1/(MPa·K^{-1})	−54.3590	−81.7111	−75.8776	−43.3746
b_2/(MPa·K^{-2})	7.5093	20.9494	18.1340	0.2285
b_3/(MPa·K^{-3})	−3.0703			−2.9669
b_4/(MPa·K^{-4})	18.2190			2.3792
T_0/K	323.15	298.15	298.15	413.17
T_{min}/K	253.15	293.15	273.15	273.15
T_{max}/K	398.15	423.20	348.15	413.17
P_{min}/MPa	0.81	0.59	1.00	0.22
P_{max}/MPa	159.51	200.00	490.33	338.01
RMSD/(kg·m^{-3})	1.241	1.157	0.486	0.641
$RMSD_r$/%	0.168	0.091	0.031	0.040
bias/(kg·m^{-3})	0.207	−0.089	0.132	−0.037
N_p	135	120	67	626
±	49	−26	17	2
s_w	0.653	0.790	0.916	0.787
ref(P_{sat})	83-mcg	83-mcg	83-mcg	83-mcg

	bromomethane	tribromomethane	iodomethane	chloroethane
c_0	0.097566	0.103492	0.095477	0.050041
b_0/MPa	69.7917	95.8169	110.8130	25.4845
b_1/(MPa·K^{-1})	−75.1337	−45.7399	−86.7987	−22.3458
b_2/(MPa·K^{-2})	37.8103		25.3188	
T_0/K	293.15	368.15	273.15	293.15
T_{min}/K	253.15	323.15	253.15	293.15
T_{max}/K	363.15	368.15	313.15	393.15
P_{min}/MPa	0.79	49.13	28.69	0.27
P_{max}/MPa	159.51	343.33	159.51	5.00
RMSD/(kg·m^{-3})	0.970	1.698	0.937	0.673
$RMSD_r$/%	0.054	0.058	0.038	0.079
bias/(kg·m^{-3})	0.118	0.014	0.014	−0.123
N_p	36	10	32	10
±	6	0	2	−4
s_w	0.806	0.194	0.634	0.396
ref(P_{sat})	86-rei/pra			83-mcg

	1,1-dichloroethane	1,2-dichloroethane	1,1,1-trichloroethane	1,1,2-trichloroethane
c_0	0.097993	0.096044	0.098723	0.099183
b_0/MPa	85.5391	99.1222	91.4677	137.2970
b_1/(MPa·K^{-1})	−71.3400	−78.1804	−70.6106	−94.7626
b_2/(MPa·K^{-2})	16.0492	17.9758	15.3800	22.6232
T_0/K	298.15	323.15	298.15	298.15
T_{min}/K	298.15	278.15	298.15	298.15
T_{max}/K	398.15	398.15	398.15	398.15
P_{min}/MPa	10.10	2.00	10.10	10.10
P_{max}/MPa	101.30	394.44	101.30	101.30
RMSD/(kg·m^{-3})	0.313	0.354	0.416	0.275
$RMSD_r$/%	0.028	0.027	0.033	0.020
bias/(kg·m^{-3})	−0.060	0.053	−0.060	−0.047
N_p	35	157	35	35
±	−1	37	1	−3
s_w	0.833	0.798	0.809	0.784
ref(P_{sat})	77-rei/pra	83-mcg	84-dyk/rep	83-mcg

	1,1,2,2-tetrachloroethane	chloroethene	*cis*-1,2-dichloroethene	*trans*-1,2-dichloroethene
c_0	0.100039	0.123720	0.069852	0.106824
b_0/MPa	167.3465	37.4817	70.0564	96.5706
b_1/(MPa·K^{-1})	−110.8381	−61.7886		100.2811
b_2/(MPa·K^{-2})		26.9744		
T_0/K	295.25	318.40	293.15	293.15
T_{min}/K	295.25	280.99	293.15	293.15
T_{max}/K	298.15	337.25	293.15	298.15[b]
P_{min}/MPa	40.53	0.38	2.00	2.00
P_{max}/MPa	459.20	4.09	10.00	101.33
RMSD/(kg·m^{-3})	0.169	0.036	0.032	0.188
$RMSD_r$/%	0.010	0.004	0.003	0.014
bias/(kg·m^{-3})	−0.011	−0.001	0.006	−0.010
N_p	14	69	5	12
±	2	3	1	−2
s_w	0.437	0.983	0.789	0.321
ref(P_{sat})		86-rei/pra		

Table 3. (Continued)

	trichloroethene	tetrachloroethene	bromoethane	1,2-dibromoethane[b]
c_0	0.100987	0.101727	0.094349	0.255137
b_0/MPa	116.0051	136.6100	89.5031	855.8329
b_1/(MPa·K^{-1})			−91.9458	-2301.0082
b_2/(MPa·K^{-2})			57.5736	
T_0/K	298.15	298.15	273.15	293.15
T_{min}/K	298.15	298.15	253.15	293.15
T_{max}/K	298.15	298.15	333.15	303.15
P_{min}/MPa	40.53	40.53	0.27	6.08
P_{max}/MPa	101.33	101.33	156.75	71.23
RMSD/(kg·m^{-3})	0.150	0.125	0.823	0.663
RMSD$_r$/%	0.010	0.007	0.055	0.030
bias/(kg·m^{-3})	−0.011	0.000	−0.044	0.276
N_p	6	7	37	7
±	0	3	−9	3
s_w	0.190	0.198	0.771	0.030
ref(P_{sat})			83-mcg	

	1-chloropropane	1-bromopropane	2-bromopropane	1-iodopropane
c_0	0.107245	0.088871	0.090158	0.101044
b_0/MPa	97.6921	94.5324	77.1648	126.9322
b_1/(MPa·K^{-1})	−83.5804	−69.6013	−52.6647	−61.3795
b_2/(MPa·K^{-2})	9.6507	15.4070	3.1100	0.8743
b_3/(MPa·K^{-3})	5.8582	−1.2323	2.3516	
T_0/K	273.15	273.15	280.00	273.15
T_{min}/K	273.15	280.00	280.00	273.15
T_{max}/K	423.15	500.00	450.00	368.15
P_{min}/MPa	0.27	5.00	5.00	49.03
P_{max}/MPa	98.07	100.00	100.00	1176.80
RMSD/(kg·m^{-3})	0.698	1.179	1.264	1.422
RMSD$_r$/%	0.078	0.094	0.100	0.070
bias/(kg·m^{-3})	−0.022	−0.091	−0.026	0.043
N_p	17	131	110	40
±	−3	−27	22	−4
s_w	0.397	0.945	1.001	0.711
ref(P_{sat})	83-mcg	Table 8	Table 8	

	1-chlorobutane	1-bromobutane	1-iodobutane	1-chloropentane
c_0	0.096363	0.097660	0.100570	0.096585
b_0/MPa	66.7185	64.6200	133.6923	72.2561
b_1/(MPa·K^{-1})	−55.2473	−46.0190	−72.9788	−54.2935
b_2/(MPa·K^{-2})	6.9367	22.4791	12.1836	23.5756
T_0/K	323.15	348.15	273.15	323.15
T_{min}/K	273.15	273.15	273.15	273.15
T_{max}/K	423.15	368.15	368.15	368.15
P_{min}/MPa	0.27	49.03	49.03	49.03
P_{max}/MPa	1176.80	1176.80	1176.80	1176.80
RMSD/(kg·m^{-3})	1.033	1.104	1.788	0.491
RMSD$_r$/%	0.102	0.074	0.091	0.046
bias/(kg·m^{-3})	0.019	0.024	−0.015	0.004
N_p	53	42	42	40
±	1	8	−8	0
s_w	0.717	0.735	0.932	0.670
ref(P_{sat})	83-mcg			

	1-bromopentane[b]	1-iodopentane	fluorobenzene	hexafluorobenzene
c_0	0.089866	0.100514	0.085382	0.084982
b_0/MPa	79.0556	133.6143	55.9961	31.6223
b_1/(MPa·K^{-1})	−60.4081	−78.9008	−51.3758	−36.1410
b_2/(MPa·K^{-2})	16.8299	18.9314	12.8141	22.4787
b_3/(MPa·K^{-3})	−2.3123		−0.8470	
T_0/K	323.15	273.15	348.15	373.10
T_{min}/K	283.00	273.15	298.15	298.11
T_{max}/K	523.00	368.15	523.15	373.18
P_{min}/MPa	5.00	49.03	2.45	0.40
P_{max}/MPa	98.10	1176.80	350.00	256.30
RMSD/(kg·m^{-3})	0.730	0.870	1.451	0.890
RMSD$_r$/%	0.061	0.049	0.148	0.053
bias/(kg·m^{-3})	−0.035	0.032	−0.356	−0.134
N_p	143	41	108	40
±	−5	5	−12	−4
s_w	0.862	0.722	0.924	0.833
ref(P_{sat})	Table 8		77-rei/pra	90-amb/ewi

Table 3. (Continued)

	chlorobenzene	1,2-dichlorobenzene	chlorocyclohexane	2,4-dichloro-1-methylbenzene
c_0	0.095711	0.093390	0.093650	0.079428
c_1(K^{-1})	−0.003690			
b_0/MPa	123.2742	140.8155	110.8746	96.0000
b_1/(MPa·K^{-1})	−81.7767	−76.8466	−111.4330	−49.5545
b_2/(MPa·K^{-2})	17.9054		−65.5947	9.3982
b_3/(MPa·K^{-3})	−1.8100			
b_4/(MPa·K^{-4})	0.1068			
T_0/K	303.15	313.14	298.15	398.00
T_{min}/K	278.15	278.15	243.15	293.00
T_{max}/K	583.15	338.13	298.15	423.00
P_{min}/MPa	0.20	2.55	10.00	10.00
P_{max}/MPa	490.33	311.51	280.00	600.00
RMSD/(kg·m^{-3})	0.562	0.209	0.672	1.290
RMSD$_r$/%	0.057	0.015	0.063	0.104
bias/(kg·m^{-3})	0.047	0.055	−0.014	−0.016
N_p	633	115	105	106
±	117	47	−5	−4
s_w	1.071	0.943	0.619	0.806
ref(P_{sat})	83-mcg			

	bromobenzene	2,4-dibromo-1-methylbenzene	iodobenzene
c_0	0.097388	0.078042	0.062476
b_0/MPa	126.5150	82.4732	77.4372
b_1/(MPa·K^{-1})	−74.1592	−53.8548	−54.5221
b_2/(MPa·K^{-2})	11.6283	2.7416	16.8124
T_0/K	323.15	398.00	348.00
T_{min}/K	278.15	293.00	293.00
T_{max}/K	358.15	423.00	423.00
P_{min}/MPa	2.50	10.00	10.00
P_{max}/MPa	280.00	600.00	600.00
RMSD/(kg·m^{-3})	0.680	2.145	3.321
RMSD$_r$/%	0.043	0.117	0.175
bias/(kg·m^{-3})	0.303	0.575	0.255
N_p	108	108	120
±	52	6	2
s_w	0.929	0.742	0.993
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] See the discussion in the text.

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 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 $P-T$ 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-type data) for a particular substance was fitted by eq 1, then average deviations of the fit (RMSD, RMSD$_r$) do not reflect a real accuracy of the experiment and consequently the weighted standard deviation, s_w, may be 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 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 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 $P-\rho-T$ 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. Values of input quantities in eq 11 were taken from different sources cited in Table 5. No comparison is presented for dibromomethane and diiodomethane (no fits were performed, see above); the isothermal compressibility values found in the literature are, however, retained in Table 5.

Two data sets available for chloromethane [64-hsu/mck, 78-kum/iwa] (see Tables 2 and 4) are in good agreement in the overlapping T,P range; the isotherms 323.15, 348.15,

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[a]

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]
				Chloromethane						
64-hsu/mck	308.15	398.15	0.8	31.6	1.382	0.188	0.283	105	47	o
78-kum/iwa	253.15	313.15	28.7	159.5	0.504	0.049	−0.057	30	2	o
				Dichloromethane						
49-bri					1.462	0.102	−1.442	4	−4	o
51-new/wea					2.507	0.181	−2.504	5	−5	o
65-sch/has					1.147	0.083	−1.129	8	−8	o
70-sch/eck					16.109	1.197	−11.358	10	−2	o
75-bur/ric	293.15	298.15	1.0	10.0	0.128	0.010	−0.104	20	−20	o
81-dic								0	0	o
82-kum/tak	298.15	348.15	10.1	101.3	0.609	0.045	−0.356	21	−11	o
85-dig/deu	343.20	423.20	10.0	200.0	1.708	0.135	−0.020	52	−2	p
85-eas/woo	298.15	298.15	50.0	100.0	0.448	0.032	−0.436	2	−2	o
91-bao/cac	298.15	298.15	0.6	102.0	0.105	0.008	0.031	25	9	p
				Trichloromethane						
49-bri	298.15	298.15	49.0	490.3	0.570	0.033	−0.130	7	−1	o
51-new/wea					2.698	0.170	−2.698	1	−1	o
51-new/wea					2.490	0.160	−2.477	6	−6	o
72-lys					52.301	3.138	−52.301	1	−1	o
75-bur/ric	293.15	298.15	1.0	10.0	0.089	0.006	−0.028	20	2	o
81-dic								0	0	o
82-kum/tak	273.15	348.15	10.8	98.7	0.670	0.043	0.416	27	19	o
84-eas/woo	298.15	298.15	50.0	250.0	0.337	0.021	0.053	5	−1	o
85-eas/woo	298.15	298.15	25.0	100.0	0.489	0.031	−0.401	3	−3	o
87-nhu/bha	293.15	293.15	2.0	10.0	0.011	0.001	0.005	5	1	o
				Tetrachloromethane						
31-bri					89.979	5.380	−73.690	9	−9	o
41-gib/loe					2.552	0.157	−1.682	20	−20	o
57-wal/ric								0	0	o
62-hol/wha	298.15	348.15	1.0	10.0	0.117	0.008	0.073	50	32	o
65-sch/has	298.15	298.15	20.0	90.0	0.363	0.022	0.139	8	2	o
69-mop	273.15	323.15	10.2	197.7	0.760	0.046	−0.396	21	−9	o
70-dic								0	0	o
73-rog/bur	298.15	298.15	1.0	10.0	0.042	0.003	−0.022	10	−2	o
75-bur/ric	293.15	298.15	1.0	10.0	0.102	0.006	−0.078	20	−18	o
76-ben/win	273.15	413.17	0.4	338.0	0.720	0.045	0.049	412	44	op
78-han/gup					1.651	0.102	1.045	24	12	p
86-eas/woo					1.907	0.114	−1.728	64	−58	o
87-hol/goe	293.15	293.15	2.0	10.0	0.027	0.002	−0.021	5	−3	o
87-lai/mil	329.81	388.26	0.2	55.7	0.546	0.036	−0.375	100	−44	e[b]
				Bromomethane						
78-kum/iwa	253.15	313.15	28.7	159.5	0.949	0.052	0.019	30	2	o
88-rut	293.15	363.15	0.8	7.0	1.066	0.065	0.608	6	4	o
				Tribromomethane						
31-bri	323.15	368.15	49.1	343.3	1.698	0.058	0.014	10	0	o
				Iodomethane						
78-kum/iwa	253.15	313.15	28.7	159.5	0.937	0.038	0.014	32	2	o
				Chloroethane						
88-rut	293.15	393.15	0.3	5.0	0.673	0.079	−0.123	10	−4	o
				1,1-Dichloroethane						
51-new/wea					1.292	0.105	−1.277	6	−6	o
85-kum/tak	298.15	398.15	10.1	101.3	0.313	0.028	−0.060	35	−1	o
				1,2-Dichloroethane						
51-new/wea					1.465	0.112	−1.453	6	−6	o
85-kum/tak	298.15	398.15	10.1	101.3	0.337	0.028	−0.169	35	−9	o
90-mal/pri					2.307	0.171	1.646	125	125	o
94-mal/woo	278.15	338.15	2.5	394.4	0.366	0.028	0.125	117	51	o
96-hah/ulc	293.15	293.15	2.0	10.0	0.089	0.007	−0.080	5	−5	o
				1,1,1-Trichloroethane						
89-kum	298.15	398.15	10.1	101.3	0.416	0.033	−0.060	35	1	o
				1,1,2-Trichloroethane						
89-kum	298.15	398.15	10.1	101.3	0.275	0.020	−0.047	35	−3	o
				1,1,2,2-Tetrachloroethane						
51-new/wea	298.15	298.15	40.5	101.3	0.198	0.012	−0.027	6	0	o
63-and	295.25	295.25	142.3	459.2	0.142	0.008	0.002	8	2	o
				Chloroethene						
82-cul/ely	280.99	337.25	0.4	4.1	0.036	0.004	−0.001	69	3	o

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]
					cis−1,2-Dichloroethene					
96-hah/ulc	293.15	293.15	2.0	10.0	0.032	0.003	0.006	5	1	o
					trans−1,2-Dichloroethene					
51-new/wea	298.15	298.15	40.5	101.3	0.246	0.019	−0.013	7	1	o
96-hah/ulc	293.15	293.15	2.0	10.0	0.008	0.001	−0.002	5	−1	o
					Trichloroethene					
51-new/wea	298.15	298.15	40.5	101.3	0.150	0.010	−0.011	6	0	o
					Tetrachloroethene					
51-new/wea	298.15	298.15	40.5	101.3	0.125	0.007	0.000	7	3	o
					Bromoethane					
42-bri								0	0	p
57-wal/ric								0	0	o
69-mil/jen					16.007	1.016	−15.219	10	−10	o
78-kum/iwa	253.15	313.15	19.7	156.8	0.740	0.049	0.070	32	−6	o
88-rut	293.15	333.15	0.3	5.0	1.228	0.088	−0.778	5	−3	o
					1,2-Dibromoethane					
60-hil/goc	293.15	293.15	6.1	42.6	0.785	0.036	0.386	5	3	o
68-ski/cus	303.15	303.15	53.4	71.2	0.001	0.000	0.000	2	0	o
					1-Chloropropane					
33-bri	273.15	368.15	49.0	98.1	1.061	0.113	0.182	5	1	o
88-rut	293.15	423.15	0.3	5.0	0.470	0.058	−0.107	12	−4	o
					1-Bromopropane					
33-bri					2.143	0.155	0.086	6	2	o
42-bri								0	0	p
71-jen/mil					10.888	0.744	−9.994	24	−24	o
78-gus/bai	280.00	500.00	5.0	100.0	1.179	0.094	−0.091	131	−27	op
88-rut					1.666	0.131	1.115	10	8	o
					2-Bromopropane					
78-gus/bai	280.00	450.00	5.0	100.0	1.264	0.100	−0.026	110	22	op
					1-Iodopropane					
33-bri	273.15	368.15	49.0	1176.8	1.422	0.070	0.043	40	−4	o
					1-Chlorobutane					
33-bri	273.15	368.15	49.0	1176.8	1.081	0.099	0.017	41	−1	o
68-ski/cus					24.880	2.431	−23.726	5	−5	o
88-rut	293.15	423.15	0.3	5.0	0.848	0.109	0.026	12	2	o
					1-Bromobutane					
33-bri	273.15	368.15	49.0	1176.8	1.104	0.074	0.024	42	8	o
42-bri					119.463	7.212	−119.36	2	−2	p
69-mil/jen					14.809	1.025	−14.156	39	−39	o
					1-Iodobutane					
33-bri	273.15	368.15	49.0	1176.8	1.788	0.091	−0.015	42	−8	o
					1-Chloropentane					
33-bri	273.15	368.15	49.0	1176.8	0.491	0.046	0.004	40	0	o
					1-Bromopentane					
33-bri					2.821	0.222	2.262	5	3	o
71-jen/mil					4.628	0.399	−2.140	28	0	o
77-gus/bai	283.00	523.00	5.0	98.1	0.730	0.061	−0.035	143	−5	op
					1-Iodopentane					
33-bri	273.15	368.15	49.0	1176.8	0.870	0.049	0.032	41	5	o
					Fluorobenzene					
74-de /fin	303.15	423.15	6.0	350.0	2.454	0.247	−1.220	33	−9	p
89-abd/akh	298.15	523.15	2.4	49.5	0.617	0.068	0.023	75	−3	op
91-ver/mel					21.572	2.046	−19.347	84	−84	op
					Hexafluorobenzene					
80-hog/kri					4.391	0.256	2.937	21	15	o
81-dym/rob	298.21	373.18	19.2	251.6	0.696	0.043	−0.226	22	−2	o
82-dym/gle	298.11	373.10	0.4	36.3	0.454	0.030	0.101	6	2	op
82-dym/gle	298.11	373.10	53.5	256.3	1.284	0.075	−0.084	12	−4	op
					Chlorobenzene					
31-bri					7.532	0.626	−6.820	13	−13	o
39-gib/loe	298.15	338.15	50.0	100.0	0.183	0.016	−0.088	6	0	o
39-gib/loe-1	298.15	358.15	25.0	100.0	0.204	0.018	−0.127	16	−10	o
42-bri								0	0	p
49-bri	298.15	298.15	49.0	490.3	0.675	0.055	−0.475	10	−8	o
63-and					1.619	0.131	−1.508	2	−2	o
68-ski/cus					6.928	0.582	−6.574	9	−9	o
70-sch/eck					5.305	0.444	−3.523	8	−4	o
73-aga/kaf	308.25	583.15	0.2	32.5	0.528	0.059	0.297	107	63	p

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]
Chlorobenzene (Continued)										
75-gus/mir					8.655	1.003	−3.888	66	−44	op
76-aga/kaf	303.15	583.15	0.3	41.9	0.620	0.069	0.061	211	9	op
80-tak					2.880	0.241	−2.573	4	−4	o
82-tak/ter	303.15	303.15	10.0	200.0	0.629	0.053	−0.450	20	−16	o
83-kas/fuk	298.15	398.15	0.2	98.2	0.779	0.069	−0.516	40	−22	o
84-abd/dzh	298.15	523.15	1.3	50.0	0.580	0.059	−0.041	74	14	p
90-won/hay	323.20	348.20	0.7	6.9	0.244	0.023	0.211	11	11	o
91-ver/mel					2.630	0.230	−0.895	112	−24	op
97-eas/bac	278.15	338.13	1.9	283.1	0.430	0.036	0.166	138	76	o
1,2-Dichlorobenzene										
97-eas/bac	278.15	338.13	2.5	311.5	0.209	0.015	0.055	115	47	o
Chlorocyclohexane										
97-jen/wue	243.15	298.15	10.0	280.0	0.672	0.063	−0.014	105	−5	o
2,4-Dichloro-1-methylbenzene										
91-ver/mel	293.00	423.00	10.0	600.0	1.290	0.104	−0.016	106	−4	o
Bromobenzene										
31-bri					1.936	0.123	−1.231	4	−2	o
39-gib/loe	298.15	338.15	50.0	100.0	0.309	0.020	−0.164	6	−2	o
39-gib/loe-1	298.15	358.15	25.0	100.0	0.274	0.018	−0.133	16	−8	o
82-tak/ter	303.15	303.15	10.0	200.0	1.521	0.097	1.456	20	20	o
87-eas/woo	278.15	323.15	2.5	280.0	0.171	0.011	0.102	66	42	o
2,4-Dibromo-1-methylbenzene										
91-ver/mel	293.00	423.00	10.0	600.0	2.145	0.117	0.575	108	6	o
Iodobenzene										
91-ver/mel	293.00	423.00	10.0	600.0	3.321	0.175	0.255	120	2	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 the reference pressure using eq 1; e, reference density values were calculated from functions given in Appendix 1. [b] See Table 7.

and 363.15 [64-hsu/mck] were, however, rejected due to large deviations. No data for isothermal compressibility were found for a comparison.

Retained data for dichloromethane resulted in a fit with the average deviation 0.09%. The deviation of the data set [85-dig/deu] is rather large (0.135%); the set was retained to enlarge the temperature range of the final fit. The average deviations of other retained data sets are below 0.05%. The agreement of calculated isothermal compressibilities with literature data (Table 5) in the temperature range from 283.15 to 313.15 K is satisfactory (the average deviation is 2.4%).

Similarly, the data sets retained for trichloromethane and tetrachloromethane deviate from the final fits (Tables 3 and 4) within 0.05% (in an average) and the agreement in isothermal compressibilities is very good (average deviations, after the extreme deviation values are excluded, are 0.7 and 1.0% for trichloromethane and tetrachloromethane, respectively). The fit for trichloromethane is, however, based predominantly on data by Kumagai and Takahashi [82-kum/tak], since the temperature ranges of other retained data sets are limited to the region close to 298.15 K. Data points of tetrachloromethane at $T = 273.15$ and $P > 45$ MPa of the retained data set [76-ben/win] were rejected due to larger deviations, similarly as some data points [87-lai/mil] around $T = 408$ K. A tentative separate fit of data [86-eas/woo] for tetrachloromethane yielded isothermal compressibilities about 3% lower than literature data, and the data [86-eas/woo] were rejected from the final fit (see large RMSD and negative bias of this data set in Table 4).

The isothermal compressibility at 275.15 K calculated from the fit of bromomethane agrees well (deviation −0.9%) with the literature value (Table 5). At this temperature range the fit is based on data by Kumagai and Iwasaki [78-kum/iwa]. No data at higher temperatures were available for a comparison, obviously due to the low normal boiling point (276 K).

The fit for tribromomethane is based on data by Bridgman [31-bri], and calculated isothermal compressibilities are more than 30% higher than literature values (Table 5). Bridgman mentioned difficulties caused by a corrosive effect of tribromomethane on brass bellows resulting even in leaks. It would be rather speculative to attribute the corrosion as a cause for tribromomethane being apparently more compressible than follows from the speed of sound, volumetric, and heat capacity data (Table 5), but on the other hand, the Bridgman values for tetrachloromethane, chlorobenzene, and bromobenzene [31-bri] obtained using the same experimental apparatus are lower than the values corresponding to the final fits (see the large negative values of bias in Table 4 which correspond to lower density and thus lower compressibility than those calculated from the fit).

The fit for iodomethane represents data by Kumagai and Iwasaki [78-kum/iwa] and yields isothermal compressibilities about 3% higher than available values from literature (Table 5).

The data set available for chloroethane [88-rut] covers the temperature interval from 293.15 to 423.15 K, but the final fit is limited up to 393.15 K, since the full-range fit resulted in distortion of the $B(T)$ function (eq 3). The value of the parameter $c_0 = 0.050\,041$ is lower than usual (ranging from 0.09 to 1.05), which may indicate that the data are rather suspect. No isothermal compressibility data were found in the literature for a comparison.

The fit of data [85-kum/tak] for 1,1-dichloroethane results in isothermal compressibility at $T = 298.15$ K less than 2% lower than the value calculated from speed-of-sound data. The values from the data set [51-new/wea] are systematically lower and were rejected. It seems obvious also that data presented by Newitt and Weale [51-new/

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)
				Dichloromethane					Tetrachloromethane (continued)
283.15	0.910[g]	0.921	−1.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	298.15	1.074 ± 0.002	1.065	0.8	83-tam/oho,[d] 96-nat,[d] 73-trc,[e] 96-zab/ruz[f]
293.15	0.989 ± 0.002	1.002	−1.3	44-sch,[d] 73-trc,[e] 96-zab/ruz[f]			1.076	−0.2	83-tam/oho,[c] 96-nat[c]
		1.000	−1.1	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.067	0.7	89-ham/man,[c] 78-kiy/hal,[d] 73-trc,[e] 96-zab/ruz[f]
		0.997	−0.8	52-jac,[d] 73-trc,[e] 96-zab/ruz[f]					
298.15	1.032 ± 0.002	1.012	2.0	51-set,[d] 73-trc,[e] 96-zab/ruz[f]			1.056	1.7	65-for/moo,[d] 73-trc,[e] 96-zab/ruz[f]
		1.08	−4.4	61-shi/hil[c]			1.070	0.4	98-ami/ban,[d] 73-trc,[e] 96-zab/ruz[f]
		1.094	−5.7	98-ami/ban,[d] 73-trc,[e] 96-zab/ruz[f]	303.15	1.119 ± 0.002	1.129	−0.9	14-tyr[c]
303.15	1.078 ± 0.003	1.088	−0.9	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.113	0.5	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]
		1.062	1.5	96-nat-1[c]			1.118	0.1	29-fre/hub[c]
		1.092	−1.2	96-nat-1,[d] 73-trc,[e] 96-zab/ruz[f]			1.108	1.0	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]
313.15	1.179 ± 0.003	1.183	−0.3	49-lag/mcm, [d]73-trc,[e] 96-zab/ruz[f]			1.128	−0.8	55-sta/tup[c]
				Trichloromethane			1.095	2.2	74-jai/nor,[d] 73-trc,[e] 96-zab/ruz[f]
273.15	0.852 ± 0.006	0.845	0.8	14-tyr[c]			1.109	0.9	80-nat/dub,[d] 73-trc, [e]96-zab/ruz[f]
		0.859	−0.8	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]			1.110	0.8	82-nat/nar,[d] 73-trc,[e] 96-zab/ruz[f]
		0.855	−0.4	29-fre/hub[c]			1.154	1.0	71-des/bha[c]
		0.854	−0.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	308.15	1.165 ± 0.002	1.162	0.3	71-des/bha,[d] 73-trc,[e] 96-zab/ruz[f]
283.15	0.920 ± 0.003	0.917	0.3	14-tyr[c]			1.223	−0.8	14-tyr[c]
		0.924	−0.4	29-fre/hub,[d] 73-trc, [e]96-zab/ruz[f]	313.15	1.213 ± 0.002	1.211	0.2	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]
		0.919	0.1	29-fre/hub[c]			1.216	−0.2	29-fre/hub[c]
		0.923	−0.3	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.206	0.6	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]
293.15	0.996 ± 0.002	0.998	−0.2	14-tyr,[c] 29-fre/hub,[d] 73-trc,[e] 96-zab/ruz,[f] 71-ric/rog[c]			1.219	−0.5	55-sta/tup[c]
							1.197	1.3	59-dia/mcg[c]
		0.994	0.2	29-fre/hub,[c] 44-sch,[d] 52-jac,[d] 73-trc,[e] 96-zab/ruz[f]			1.191	1.8	66-kat/shi[c]
							1.203	0.8	80-nat/dub,[d] 73-trc,[e] 96-zab/ruz[f]
		1.000	−0.4	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.245	1.4	71-des/bha[c]
		0.997	−0.1	52-jac[c]	318.15	1.263 ± 0.002	1.265	−0.2	71-des/bha,[d] 73-trc,[e] 96-zab/ruz[f]
		1.015	−1.9	55-sta/tup,[c] 87-abd/mun[c]			1.332	−1.3	14-tyr[c]
		1.040	−4.4	68-day[c]	323.15	1.315 ± 0.002	1.320	−0.4	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]
298.15	1.037 ± 0.002	1.041	−0.4	65-for/moo,[d] 73-trc,[e] 96-zab/ruz[f]			1.326	−0.8	29-fre/hub[c]
		1.039	−0.2	87-aka/oga,[d] 73-trc,[e] 96-zab/ruz[f]			1.315	0.0	49-lag/mcm,[d] 73-trc, [e]96-zab/ruz[f]
		1.038	−0.1	98-ami/ban,[d] 73-trc,[e] 96-zab/ruz[f]			1.320	−0.4	55-sta/tup[c]
		0.994	4.3	98-ami/pat,[d] 73-trc,[e] 96-zab/ruz[f]			1.352	−2.7	59-dia/mcg[c]
298.25	1.081 ± 0.002	1.041	−0.3	54-gab/poi,[d] 73-trc,[e] 96-zab/ruz[f]			1.309	0.5	66-kat/shi[c]
303.15	1.081 ± 0.003	1.086	−0.5	14-tyr[c]			1.452	−1.7	14-tyr[c]
		1.080	0.1	29-fre/hub,[d] 49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	333.15	1.428 ± 0.002	1.437	−0.6	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]
		1.081	0.0	29-fre/hub[c]			1.425	0.2	55-sta/tup[c]
		1.098	−1.5	55-sta/tup[c]			1.420	0.6	66-kat/shi[c]
		1.079	0.2	80-nat/dub,[d] 73-trc,[e] 96-zab/ruz[f]	343.15	1.553 ± 0.003	1.577	−1.5	14-tyr[c]
313.15	1.178 ± 0.006	1.184	−0.5	14-tyr[c]			1.543	0.6	55-sta/tup[c]
		1.236	−4.7	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]			1.565	−0.8	66-kat/shi[c]
		1.179	−0.1	29-fre/hub[c]	349.09	1.635 ± 0.003	1.652	−1.0	79-bob/nie,[d] 73-trc,[e] 96-zab/ruz[f]
		1.171	0.6	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]					Bromomethane
		1.193	−1.3	55-sta/tup[c]	275.15	1.153 ± 0.014	1.163	−0.9	46-pel/gal,[d] 80-trc,[e] 96-zab/ruz[f]
		1.167	0.9	80-nat/dub,[d] 73-trc,[e] 96-zab/ruz[f]					Dibromomethane
323.15	1.286 ± 0.008	1.290	−0.3	14-tyr[c]	273.15	–	0.556	–	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
		1.270	1.3	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	283.15	–	0.599	–	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
		1.295	−0.7	55-sta/tup[c]	293.15	–	0.644	–	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
333.15	1.409 ± 0.009	1.406	0.2	14-tyr[c]	298.15	–	0.675	–	51-set,[d] 80-trc,[e] 96-zab/ruz[f]
				Tetrachloromethane	303.15	–	0.692	–	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
273.15	0.877 ± 0.006	0.898	−2.3	14-tyr[c]					Tribromomethane
		0.860	2.0	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]	293.15	0.795[g]	0.557	42.7	29-fre/hub,[d] 44-sch,[d] 80-trc,[e] 96-zab/ruz[f]
		0.885	−0.9	29-fre/hub[c]					
		0.867	1.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			0.554	43.5	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
283.15	0.951 ± 0.003	0.970	−2.0	14-tyr[c]	298.15	0.809[g]	0.571	41.7	93-ami/rai,[d] 80-trc,[e] 96-zab/ruz[f]
		0.940	1.2	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]			0.564	43.4	98-ami/pat,[d] 80-trc,[e] 96-zab/ruz[f]
		0.957	−0.6	29-fre/hub[c]	303.15	0.824[g]	0.591	39.4	29-fre/hub,[d] 80-trc,[e] 96-zab/ruz[f]
		0.940	1.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			0.588	40.1	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
		0.944	0.7	59-dia/mcg[c]	313.15	0.855[g]	0.628	36.1	29-fre/hub,[d] 80-trc,[e] 96-zab/ruz[f]
293.15	1.032 ± 0.002	1.046	−1.3	14-tyr[c]			0.626	36.6	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
		1.024	0.8	29-fre/hub,[d] 73-trc,[e] 96-zab/ruz[f]	323.15	0.888 ± 0.016	0.668	32.9	29-fre/hub,[d] 80-trc,[e] 96-zab/ruz[f]
		1.034	−0.2	29-fre/hub[c]			0.666	33.3	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
		1.020	1.2	44-sch,[d] 49-lag/mcm,[d] 82-nat/nar,[d] 73-trc,[e] 96-zab/ruz[f]	333.15	0.925 ± 0.016	0.709	30.5	49-lag/mcm,[d] 80-trc,[e] 96-zab/ruz[f]
									Iodomethane
		1.037	−0.5	52-jac[c]	275.15	0.874 ± 0.010	0.850	2.8	46-pel/gal,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		1.021	1.1	52-jac,[d] 73-trc,[e] 96-zab/ruz[f]	293.15	1.001 ± 0.012	0.981	2.0	44-sch,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		1.040	−0.8	55-sta/tup[c]			0.984	1.7	52-jac,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		1.026	0.6	79-ern/gli,[d] 73-trc,[e] 96-zab/ruz[f]	303.15	1.096 ± 0.014	1.042	5.2	46-pel/gal,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		1.060	−2.6	87-abd/mun[c]					Diiodomethane
		1.023	0.8	97-nat,[d] 73-trc,[e] 96-zab/ruz[f]	293.15	–	0.427	–	52-jac,[d] 60-grz/jef,[e] 96-zab/ruz[f,g]
		1.033	−0.1	97-nat[c]	298.15	–	0.432	–	51-set,[d] 60-grz/jef,[e] 96-zab/ruz[f,g]
298.15	1.074 ± 0.002	1.059	1.4	59-dia/mcg[c]	303.15	–	0.443	–	49-lag/mcm,[d] 60-grz/jef,[e] 96-zab/ruz[f]
		1.073	0.1	71-des/bha[c]	313.15	–	0.465	–	49-lag/mcm,[d] 60-grz/jef,[e] 96-zab/ruz[f]
		1.069	0.5	71-des/bha,[d] 73-trc,[e] 96-zab/ruz[f]	323.15	–	0.488	–	49-lag/mcm,[d] 60-grz/jef,[e] 96-zab/ruz[f]
		1.078	−0.4	78-kiy/hal[c]	333.15	–	0.514	–	49-lag/mcm,[d] 60-grz/jef,[e] 96-zab/ruz[f]
		1.075	−0.1	78-gro/wil[c]					
		1.064	0.9	78-gro/wil,[d] 89-nar/swa,[d] 73-trc,[e] 96-zab/ruz[f]					

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)
		1,1-Dichloroethane					Trichloroethene		
298.15	1.144 ± 0.007	1.160	−1.4	51-set,[d] 73-trc,[e] 96-zab/ruz[f]	298.15	0.870 ± 0.007	0.924	−5.8	extrapolated
		1.167	−2.0	51-set,[d] 85-kum/tak,[e] 96-zab/ruz[f]	303.15	–	0.965	–	80-nat/dub,[d] 96-kri/sur,[d] 97-ven/ven,[d] 99-ilo/par,[d] 90-fra/com,[e] 96-zab/ruz[f,g]
		1,2-Dichloroethane					0.956	–	96-nat-1[c]
273.15	0.673[g]	0.691	−2.6	14-tyr[c]			1.033	–	80-nat/dub,[d] 90-fra/com,[e] 96-zab/ruz[f,g]
		0.673	0.0	49-lag/mcm,[d] 93-cda,[e] 96-zab/ruz[f]	313.15	–			
		0.666	1.1	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			Tetrachloroethene		
283.15	0.720 ± 0.002	0.742	−3.0	14-tyr[c]	293.15	–	0.781	–	82-nat/nar,[d] 91-com/fra,[e,g] 96-zab/ruz[f]
		0.726	−0.8	49-lag/mcm,[d] 73-trc,[e] 93-cda,[e] 96-zab/ruz[f]	298.15	0.744 ± 0.006	0.797	−6.6	interpolated
293.15	0.773 ± 0.002	0.797	−3.0	14-tyr[c]	303.15	–	0.809	–	82-nat/nar,[d] 91-com/fra,[e] 96-zab/ruz[f]
		0.781	−1.0	44-sch,[d] 49-lag/mcm,[d] 93-cda,[e] 96-zab/ruz[f]			0.825	–	96-nat-1[c]
							0.802	–	96-kri/sur,[d] 91-com/fra,[e] 96-zab/ruz[f]
		0.782	−1.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			Bromoethane		
		0.783	−1.3	55-sta/tup[c]	273.15	1.053 ± 0.012	1.076	−2.1	14-tyr[c]
298.15	0.801 ± 0.002	0.781	2.6	51-set,[d] 93-cda,[e] 96-zab/ruz[f]			1.103	−4.5	49-lag/mcm,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		0.805	−0.5	65-for/moo,[d] 93-cda,[e] 96-zab/ruz[f]					
303.15	0.831 ± 0.002	0.858	−3.1	14-tyr[c]	275.15	1.075 ± 0.012	1.124	−4.4	46-pel/gal,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		0.845	−1.7	49-lag/mcm,[d] 93-cda,[e] 96-zab/ruz[f]	283.15	1.165 ± 0.015	1.178	−1.1	14-tyr[c]
		0.841	−1.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.197	−2.7	46-pel/gal,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		0.842	−1.3	55-sta/tup[c]			1.192	−2.3	49-lag/mcm,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		0.846	−1.7	96-kri/sur,[d] 93-cda,[e] 96-zab/ruz[f]					
		0.842	−1.3	96-kri/sur,[d] 73-trc,[e] 96-zab/ruz[f]	293.15	1.283 ± 0.017	1.295	−0.9	14-tyr[c]
		0.848	−2.0	96-nat-1[c]			1.293	−0.8	49-lag/mcm,[d] 78-kum/iwa,[e] 96-zab/ruz[f]
		0.843	−1.4	96-nat-2,[d] 73-trc,[e] 96-zab/ruz[f]					
313.15	0.896 ± 0.002	0.925	−3.1	14-tyr[c]			1.292	−0.7	52-jac[c]
		0.913	−1.9	49-lag/mcm,[d] 93-cda,[e] 96-zab/ruz[f]	303.15	1.404 ± 0.020	1.423	−1.3	14-tyr[c]
		0.893	0.3	49-lag/mcm,[d] 73-trc, [e]96-zab/ruz[f]	313.15[i]	1.521 ± 0.022	1.552	−2.0	14-tyr[c]
		0.910	−1.5	55-sta/tup[c]			1,2-Dibromoethane		
323.15	0.968 ± 0.003	0.999	−3.1	14-tyr[c]	288.15	0.263[g]	0.610	−56.9	80-aoi/ara[c]
		0.986	−1.8	55-sta/tup,[c] 49-lag/mcm,[d] 93-cda,[e] 96-zab/ruz[f]	293.15	0.298 ± 0.010	0.613	−51.4	49-lag/mcm,[d,e] 96-zab/ruz[f]
							0.627	−52.5	80-aoi/ara[c]
		0.938	3.1	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	298.15	0.344 ± 0.007	0.645	−46.7	80-aoi/ara[c]
333.15	1.049 ± 0.003	1.083	−3.1	14-tyr[c]	303.15	0.408 ± 0.003	0.658	−38.0	49-lag/mcm,[d,e] 96-zab/ruz[f]
		1.068	−1.8	55-sta/tup[c]			0.663	−38.5	80-aoi/ara[c]
343.15	1.139 ± 0.004	1.176	−3.1	14-tyr[c]	308.15	0.500[g]	0.683	−26.8	80-aoi/ara[c]
		1.156	−1.5	55-sta/tup[c]	313.15	0.645[g]	0.708	−8.9	49-lag/mcm,[d,e] 96-zab/ruz[f]
353.15	1.241 ± 0.004	1.279	−3.0	14-tyr[c]			0.703	−8.3	80-aoi/ara[c]
		1,1,1-Trichloroethane			318.15	0.909[g]	0.723	25.7	80-aoi/ara[c]
303.15	1.121 ± 0.008	1.174	−4.5	96-kri/sur,[d] 73-trc,[e] 96-zab/ruz[f]			1-Chloropropane		
		1.193	−6.0	96-kri/sur,[d] 89-kum,[e] 96-zab/ruz[f]	275.15	1.116 ± 0.036	1.203	−7.2	46-pel/gal,[d] 81-trc,[e] 96-zab/ruz[f]
		1,1,2-Trichloroethane			288.15	1.254 ± 0.040	1.313	−4.5	81-aoi/ara[c]
288.15	0.674[g]	0.704	−4.3	80-aoi/ara[c]			1.288	−2.6	81-aoi/ara,[d,e] 96-zab/ruz[f]
293.15	0.698[g]	0.726	−3.9	80-aoi/ara[c]			1.318	−4.9	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
298.15	0.722 ± 0.004	0.749	−3.6	80-aoi/ara[c]	293.15	1.316 ± 0.042	1.340	−1.8	44-sch,[d] 81-trc,[e] 96-zab/ruz[f]
303.15	0.747 ± 0.004	0.773	−3.4	80-aoi/ara[c]			1.342	−1.9	52-jac,[d] 81-trc,[e] 96-zab/ruz[f]
308.15	0.774 ± 0.004	0.799	−3.1	80-aoi/ara[c]			1.363	−3.4	81-aoi/ara[c]
313.15	0.802 ± 0.004	0.825	−2.8	80-aoi/ara[c]			1.346	−2.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
318.15	0.831 ± 0.005	0.852	−2.5	80-aoi/ara[c]			1.373	−4.2	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
		1,1,2,2-Tetrachloroethane			298.15	1.382 ± 0.046	1.413	−2.2	81-aoi/ara[c]
273.15	–	0.564	–	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.405	−1.6	81-aoi/ara,[d,e] 96-zab/ruz[f]
283.15	–	0.598	–	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.428	−3.2	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
288.15	–	0.603	–	81-aoi/ara[c]	303.15	1.454 ± 0.050	1.470	−1.1	81-aoi/ara[c]
		0.623	–	81-aoi/ara,[d,e] 96-zab/ruz[f]			1.472	−1.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.620	–	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.491	−2.5	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
293.15	0.589[g]	0.636	−7.4	44-sch,[d] 73-trc,[e] 96-zab/ruz[f]	308.15	1.533 ± 0.054	1.525	0.5	81-aoi/ara[c]
		0.637	−7.5	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]			1.536	−0.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.620	−5.0	81-aoi/ara[c]			1.550	−1.1	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
		0.641	−8.1	81-aoi/ara,[d,e] 96-zab/ruz[f]	313.15	1.618 ± 0.061	1.587	2.0	81-aoi/ara[c]
		0.640	−8.0	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.613	0.3	81-aoi/ara,[d,e] 96-zab/ruz[f]
295.25	0.597 ± 0.002	0.643	−7.2	interpolated			1.621	−0.2	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
298.15	0.609 ± 0.003	0.638	−4.5	81-aoi/ara[c]	318.15	1.711 ± 0.068	1.654	3.4	81-aoi/ara[c]
		0.660	−7.7	81-aoi/ara,[d,e] 96-zab/ruz[f]			1.691	1.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.661	−7.9	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.694	1.0	81-aoi/ara,[d] 81-trc,[e] 96-zab/ruz[f]
		0.659	−7.6	83-nat/tri,[d] 73-trc,[e] 96-zab/ruz[f]			1-Bromopropane		
303.15	0.630[g]	0.679	−7.2	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	275.15	0.953[g]	0.943	1.1	46-pel/gal,[d] 88-rut,[e,g] 78-gus/bai,[e,g] 96-zab/ruz[f]
		0.656	−4.0	81-aoi/ara[c]					
		0.680	−7.4	81-aoi/ara,[d,e] 96-zab/ruz[f]	288.15	1.051 ± 0.010	1.056	−0.5	81-aoi/ara[c]
		0.682	−7.6	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.040	−1.1	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.683	−7.8	96-kri/sur,[d] 73-trc,[e] 96-zab/ruz[f]			1.049	−0.2	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
		0.686	−8.2	96-nat-2[c]					
308.15	–	0.676	–	81-aoi/ara[c]	293.15	1.093 ± 0.010	1.092	0.1	81-aoi/ara[c]
		0.700	–	81-aoi/ara,[d,e] 96-zab/ruz[f]			1.085	0.7	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.704	–	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.094	−0.1	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
		0.702	–	83-nat/tri,[d] 73-trc,[e] 96-zab/ruz[f]					
313.15	–	0.723	–	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]	298.15	1.137 ± 0.010	1.129	0.7	81-aoi/ara[c]
		0.695	–	81-aoi/ara[c]			1.131	0.5	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.721	–	81-aoi/ara,[d,e] 96-zab/ruz[f]			1.140	−0.3	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
		0.727	–	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]					
318.15	–	0.716	–	81-aoi/ara[c]	303.15	1.183 ± 0.010	1.168	1.3	81-aoi/ara[c]
		0.743	–	81-aoi/ara,[d,e] 96-zab/ruz[f]			1.181	0.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		0.751	–	81-aoi/ara,[d] 73-trc,[e] 96-zab/ruz[f]			1.190	−0.6	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
323.15	–	0.773	–	49-lag/mcm,[d] 73-trc,[e] 96-zab/ruz[f]					

Table 5. (Continued)

T/K	β_T/GPa^{-1} eq 1[a]	β_T/GPa^{-1} lit.	$\delta\beta_T$[b]/%	ref(s)
		1-Bromopropane (continued)		
308.15	1.232 ± 0.010	1.210	1.8	81-aoi/ara[c]
		1.234	−0.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		1.244	−1.0	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
313.15	1.285 ± 0.010	1.252	2.6	81-aoi/ara[c]
		1.288	−0.2	81-aoi/ara,[d,e] 96-zab/ruz[f]
		1.298	−1.0	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
318.15	1.340 ± 0.010	1.297	3.3	81-aoi/ara[c]
		1.346	−0.4	81-aoi/ara,[d,e] 96-zab/ruz[f]
		1.356	−1.2	81-aoi/ara,[d] 88-rut,[e] 78-gus/bai,[e] 96-zab/ruz[f]
		2-Bromopropane		
293.15	1.281 ± 0.013	1.271	0.8	87-abd/mun[e]
		1-Iodopropane		
293.15	0.880 ± 0.007	0.90	−2.2	44-sch,[d] 43-vog,[e], 96-zab/ruz[f,g]
		1-Chlorobutane		
293.15	1.147 ± 0.011	1.166	−1.6	44-sch,[d] 81-trc,[e] 96-zab/ruz[f]
		1.156	−0.8	49-lag/mcm,[d] 81-trc,[e] 96-zab/ruz[f]
298.15	1.189 ± 0.012	1.213	−2.0	91-mat/tar,[c] 95-pic/men[c]
		1.210	−1.7	00-dom/laf,[d] 81-trc,[e] 96-zab/ruz[f]
303.15	1.233 ± 0.013	1.259	−2.1	49-lag/mcm,[d] 81-trc,[e] 96-zab/ruz[f]
308.15	1.280 ± 0.014	1.284	−0.3	95-pic/men[c]
313.15	1.331 ± 0.015	1.394	−4.5	00-dom/laf,[d,f,h] 81-trc[e]
318.15	1.385 ± 0.016	1.435	−3.5	91-mat/tar[c]
		1-Bromobutane		
293.15	1.009 ± 0.008	1.02	−1.1	44-sch,[d] 43-vog,[e], 96-zab/ruz[f]
		0.979	3.1	49-lag/mcm,[d] 43-vog,[e] 96-zab/ruz[f]
		1.003	0.6	49-lag/mcm,[d,e] 96-zab/ruz[f]
298.15	1.046 ± 0.008	1.026	1.9	83-dia/lai,[c] 83-dia/lai-1[c]
303.15	1.085 ± 0.008	1.060	2.4	49-lag/mcm,[d] 43-vog,[e] 96-zab/ruz[f]
		1.084	0.1	49-lag/mcm,[d,e] 96-zab/ruz[f]
308.15	1.126 ± 0.009	1.107	1.7	83-dia/lai,[c] 83-dia/lai-1[c]
313.15	1.168 ± 0.010	1.149	1.7	49-lag/mcm,[d] 43-vog,[e] 96-zab/ruz[f]
		1.174	−0.5	49-lag/mcm,[d,e] 96-zab/ruz[f]
318.15	1.212 ± 0.010	1.198	1.2	83-dia/lai,[c] 83-dia/lai-1[c]
323.15	1.258 ± 0.011	1.249	0.7	49-lag/mcm,[d] 43-vog,[e] 96-zab/ruz[f]
		1.274	−1.3	49-lag/mcm,[d,e] 96-zab/ruz[f]
333.15	1.354 ± 0.012	1.350	0.3	83-dia/lai,[c] 83-dia/lai-1[c]
		1-Chloropentane		
298.15	1.105 ± 0.005	1.093	1.1	95-pic/men[c]
308.15	1.192 ± 0.006	1.181	0.9	95-pic/men[c]
		1-Bromopentane		
293.15	0.909 ± 0.006	1.05	−13.4	44-sch,[d] 52-jac,[d] 43-vog,[e] 96-zab/ruz[f,g]
		1.09	−16.6	44-sch,[d] 52-jac,[d] 77-gus/bai,[e] 96-zab/ruz[f,g]
		Fluorobenzene		
273.15	0.836[g]	0.834	0.2	49-lag/mcm,[d] 89-abd/akh,[e] 96-zab/ruz[f]
283.15	0.898[g]	0.897	0.1	49-lag/mcm,[d] 89-abd/akh,[e] 96-zab/ruz[f]
293.00	0.965[g]	0.968	−0.3	91-ver/mel,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.063	−9.2	91-ver/mel,[d,e] 96-zab/ruz[f]
293.15	0.966[g]	0.938	3.0	49-lag/mcm,[d,e] 96-zab/ruz[f]
		0.964	0.2	49-lag/mcm,[d] 52-jac,[d] 89-abd/akh,[e] 96-zab/ruz[g]
		0.968	−0.2	77-lan/mue,[d] 89-abd/akh,[e] 96-zab/ruz[g]
		0.930	3.9	77-lan/mue[c]
303.00	1.041 ± 0.014	1.041	0.0	91-ver/mel,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.116	−6.7	91-ver/mel,[d,e] 96-zab/ruz[f]
303.15	1.043 ± 0.014	1.040	0.3	49-lag/mcm,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.021	2.2	49-lag/mcm,[d,e] 96-zab/ruz[f]
		1.033	1.0	88-tak,[d] 89-abd/akh,[e] 96-zab/ruz[g]
313.15	1.128 ± 0.013	1.121	0.6	49-lag/mcm,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.110	1.6	49-lag/mcm,[d,e] 96-zab/ruz[f]
323.00	1.223 ± 0.013	1.217	0.5	91-ver/mel,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.237	−1.1	91-ver/mel,[d,e] 96-zab/ruz[f]
323.15	1.224 ± 0.013	1.217	0.6	49-lag/mcm,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.215	0.7	49-lag/mcm,[d,e] 96-zab/ruz[f]
		1.218	0.5	77-lan/mue,[d] 89-abd/akh,[e] 96-zab/ruz[f]
348.00	1.520 ± 0.012	1.502	1.2	91-ver/mel,[d] 89-abd/akh,[e] 96-zab/ruz[f]
		1.420	7.0	91-ver/mel,[d,e] 96-zab/ruz[f]
		Hexafluorobenzene		
298.15	1.190 ± 0.010	1.204	−1.2	74-ski/stu[c]
		1.214	−2.0	77-mas/nor,[i] 74-hal/tow[e]
		1.227	−3.0	77-mas/nor,[d] 74-hal/tow,[e] 96-zab/ruz[f]
308.15	1.314 ± 0.010	1.276	3.0	77-mas/nor,[i] 74-hal/tow[e]
		1.354	−3.0	77-mas/nor,[d] 74-hal/tow,[e] 96-zab/ruz[f]
318.15	1.456 ± 0.010	1.471	−1.0	77-mas/nor,[d] 74-hal/tow,[e] 96-zab/ruz[f]
		Chlorobenzene		
273.15	0.647[g]	0.661	−2.1	14-tyr[c]
		0.634	2.1	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
283.15	0.687 ± 0.002	0.702	−2.1	14-tyr[c]
		0.679	1.2	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
293.00	0.729 ± 0.002	0.732	−0.4	91-ver/mel,[d] 90-trc,[e] 96-zab/ruz[f]
293.15	0.729 ± 0.002	0.743	−1.9	14-tyr[c]
		0.731	−0.3	29-fre/hub,[d] 90-trc,[e] 96-zab/ruz[f]
		0.738	−1.2	29-fre/hub[c]
		0.727	0.3	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
		0.724	0.7	52-jac,[d] 90-trc,[e] 96-zab/ruz[f]
		0.731	−0.3	68-day[c]
		0.742	−1.8	71-ric/rog[c]
		0.729	0.0	77-lan/mue,[d] 94-tak,[d] 90-trc,[e] 96-zab/ruz[f]
		0.739	−1.4	77-lan/mue[c]
		0.715	2.0	87-abd/mun[c]
298.15	0.752 ± 0.002	0.771	−2.5	71-des/bha[c]
		0.758	−0.8	71-des/bha,[d] 90-trc,[e] 96-zab/ruz[f]
		0.755	−0.4	94-tak,[d] 90-trc,[e] 96-zab/ruz[f]
		0.768	−2.1	97-oho/tam[c]
		0.750	0.3	97-oho/tam,[d] 90-trc,[e] 96-zab/ruz[f]
303.00	0.775 ± 0.002	0.781	−0.8	91-ver/mel,[d] 90-trc,[e] 96-zab/ruz[f]
303.15	0.776 ± 0.002	0.788	−1.5	14-tyr[c]
		0.783	−0.9	29-fre/hub,[d] 90-trc,[e] 96-zab/ruz[f]
		0.784	−1.0	29-fre/hub[c]
		0.782	−0.8	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
		0.780	−0.5	88-tak,[d] 90-trc,[e] 96-zab/ruz[f]
		0.781	−0.6	94-tak,[d] 90-trc,[e] 96-zab/ruz[f]
308.15	0.801 ± 0.002	0.821	−2.4	71-des/bha[c]
		0.814	−1.6	71-des/bha,[d] 90-trc,[e] 96-zab/ruz[f]
313.15	0.826 ± 0.002	0.839	−1.5	14-tyr[c]
		0.838	−1.4	29-fre/hub,[d] 94-tak,[d] 90-trc,[e] 96-zab/ruz[f]
		0.832	−0.7	29-fre/hub[c]
		0.837	−1.3	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
318.15	0.853 ± 0.002	0.876	−2.6	71-des/bha[c]
		0.874	−2.4	71-des/bha,[d] 90-trc,[e] 96-zab/ruz[f]
323.00	0.881 ± 0.002	0.902	−2.3	91-ver/mel,[d]90-trc,[e]96-zab/ruz[f]
323.15	0.882 ± 0.002	0.892	−1.1	14-tyr[c]
		0.897	−1.7	29-fre/hub,[d] 90-trc,[e] 96-zab/ruz[f]
		0.883	−0.1	29-fre/hub[c]
		0.900	−2.0	49-lag/mcm,[d] 77-lan/mue,[d] 94-tak,[d] 90-trc,[e] 96-zab/ruz[f]
333.15	0.942 ± 0.002	0.950	−0.8	14-tyr[c]
		0.966	−2.5	49-lag/mcm,[d] 90-trc,[e] 96-zab/ruz[f]
343.15	1.009 ± 0.002	1.013	−0.4	14-tyr[c]
348.00	1.043 ± 0.002	1.079	−3.3	91-ver/mel,[d] 90-trc,[e] 96-zab/ruz[f]
353.15	1.082 ± 0.002	1.079	−0.3	14-tyr[c]
373.00	1.252 ± 0.003	1.301	−3.8	91-ver/mel,[d] 90-trc,[e] 96-zab/ruz[f]
398.00	1.525 ± 0.004	1.571	−2.9	91-ver/mel,[d] 90-trc,[e] 96-zab/ruz[f]
		1,2-Dichlorobenzene		
303.15	0.628 ± 0.001	0.652	−3.7	96-sek/nai,[d] 90-trc,[e] 96-zab/ruz[f]
		Chlorocyclohexane		
293.15	0.805 ± 0.010	0.768	4.8	44-sch,[d,e] 93-cda,[e] 99-rod/laf[f,g]
298.15	0.844 ± 0.011	0.790	6.8	99-rod/laf[c]
313.15	1.009[g]	0.868	16.2	99-rod/laf[c]
		Bromobenzene		
283.15	0.616 ± 0.002	0.584	5.5	49-lag/mcm,[d,e] 96-zab/ruz[f]
293.15	0.650 ± 0.002	0.639	1.7	49-lag/mcm,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]
		0.635	2.4	49-lag/mcm,[d,e] 96-zab/ruz[f]
		0.656	−0.9	52-jac,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]
		0.628	3.5	68-day[c]
		0.650	0.0	77-lan/mue,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]
		0.651	−0.2	77-lan/mue[d]
		0.621	4.7	87-abd/mun[c]
		0.649	0.2	94-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]

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)
	Bromobenzene (continued)					Iodobenzene			
298.15	0.668 ± 0.002	0.669	−0.1	94-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]	283.15	0.521[g]	0.550	−2.3	49-lag/mcm,[d,e] 96-zab/ruz[f]
303.15	0.686 ± 0.002	0.690	−0.6	49-lag/mcm,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]	293.00	0.555 ± 0.012	0.583	−4.8	91-ver/mel,[d] 49-lag/mcm,[e] 96-zab/ruz[f]
		0.692	−0.9	49-lag/mcm,[d,e] 96-zab/ruz[f]			0.592	−6.3	91-ver/mel,[d] 65-mal/hil,[e] 96-zab/ruz[f]
		0.691	−0.7	82-ven/dha,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]			0.565	−1.8	91-ver/mel,[d,e] 96-zab/ruz[f]
					293.15	0.555 ± 0.012	0.582	−4.6	49-lag/mcm,[d,e] 96-zab/ruz[f]
		0.684	0.3	88-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]	303.00	0.592 ± 0.012	0.616	−3.9	91-ver/mel,[d] 49-lag/mcm,[e] 96-zab/ruz[f]
		0.690	−0.6	94-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]					
313.15	0.726 ± 0.002	0.735	−1.2	49-lag/mcm,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]			0.630	−6.0	91-ver/mel,[d] 65-mal/hil,[e] 96-zab/ruz[f]
							0.599	−1.2	91-ver/mel,[d,e] 96-zab/ruz[f]
		0.756	−4.0	49-lag/mcm,[d,e] 96-zab/ruz[f]	303.15	0.593 ± 0.012	0.616	−3.7	49-lag/mcm,[d,e] 96-zab/ruz[f]
		0.735	−1.2	94-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]	313.15	0.634 ± 0.012	0.651	−2.6	49-lag/mcm,[d,e] 96-zab/ruz[f]
323.15	0.769 ± 0.002	0.783	−1.8	49-lag/mcm,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]	323.00	0.677 ± 0.013	0.691	−2.0	91-ver/mel,[d] 49-lag/mcm,[e] 96-zab/ruz[f]
		0.784	−1.9	77-lan/mue,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]			0.677	0.0	91-ver/mel,[d,e] 96-zab/ruz[f]
					323.15	0.678 ± 0.013	0.689	−1.6	49-lag/mcm,[d,e] 96-zab/ruz[f]
		0.782	−1.7	94-tak,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]					
333.15	0.816 ± 0.001	0.834	−2.2	49-lag/mcm,[d] 39-gib/loe-1,[e] 96-zab/ruz[f]					

[a] Uncertainty is estimated as ±2s, where s is a standard deviation derived from a covariance matrix of each fit. [b] $[\beta_T(\text{eq 1}) - \beta_T(\text{lit})] \times 100/\beta_T(\text{lit})$. [c] Isothermal compressibility, $\beta_T = (1/\rho)(\partial\rho/\partial P)_T = -(1/V)(\partial V/\partial P)_T$. [d] Sound speed. [e] Density and thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$. [f] Isobaric heat capacity. [g] Extrapolated. [h] Cited value of heat capacity used. [i] Normal boiling temperature 311.5 K, β_T was calculated for $P = 0.1$ MPa, not for saturation pressure. [j] Thermal pressure coefficient, $\gamma_V = (\partial P/\partial T)_V$; β_T was obtained as $\beta_T = \alpha_P/\gamma_V$.

Table 6. Comparison of Group-Contribution Volume-Ratio Method (GCVRM) Predictions with Experimental Values of Chloroalkanes Retained for the Fits in Table 3

			P_{max}	$\delta_r(V_r)$[a]	$\delta_{r,max}(V_r)$[b]
	N_p	T_r-range	MPa	%	%
chloromethane	135	0.61−0.96	159.5	4.57	19.38
dichloromethane	120	0.57−0.83	200.0	0.92	2.94
	105		150.0	0.67	2.41
trichloromethane	67	0.51−0.65	490.3	0.14	0.45
	59		150.0	0.10	0.40
tetrachloromethane	626	0.49−0.74	338.0	0.36	1.45
	554		150.0	0.23	0.99
chloroethane	10	0.64−0.85	5.0	0.54	1.47
1,1-dichloroethane	35	0.57−0.76	101.3	0.68	1.61
1,2-dichloroethane	157	0.50−0.71	394.4	0.69	−1.10
	110		150.0	0.49	−0.90
1,1,1-trichloroethane	35	0.55−0.73	101.3	0.08	−0.25
1,1,2-trichloroethane	35	0.56−0.75	101.3	2.91	−5.51
1,1,2,2-tetrachloroethane	14	0.47	459.2	1.78	−2.29
	7		150.0	1.23	−1.65
1-chloropropane	17	0.54−0.84	98.1	1.09	3.87
1-chlorobutane	53	0.51−0.79	1176.8	0.79	1.86
	21		150.0	0.20	0.56
1-chloropentane	40	0.48−0.65	1176.8	0.72	1.26
	8		150.0	0.53	−1.09

[a] $\delta_r(V_r)/\% = 100\{\Sigma_i\ [V_r(\text{GCVRM})_i/V_r(\text{exp})_i - 1]^2/N_p\}^{1/2}$; $V_r = V(T,P)/V(T,P_{ref}) = \rho(T,P_{ref})/\rho(T,P)$. [b] $\delta_{r,max}(V_r) = 100[V_r(\text{GCVRM})_i/V_r(\text{exp})_i - 1]$ corresponds to the maximum absolute value of $100[V_r(\text{GCVRM})_i/V_r(\text{exp})_i - 1]$, $i = 1, ..., N_p$.

wea] for other liquids (dichloromethane, trichloromethane, 1,2-dichloromethane; see Table 4) exhibit negative deviations from other retained data.

Retained data sets for 1,2-dichloroethane are in very good mutual agreement. Similarly as in the cases of dichloromethane, trichloromethane, and 1,1-dichloromethane, the data [51-new/wea] were rejected due to large negative deviations. The other rejected data set [90-mal/pri] represents the values calculated from a smoothing function (F-data), and the values are higher than those published later by the same laboratory [94-mal/woo]. The agreement between isothermal compressibilities calculated from the fit and literature values is quite satisfactory (Table 5); the deviations are, however, mostly negative. The highest deviations (−3%) are observed for values reported by Tyrer [14-tyr].

The fits for 1,1,1-trichloroethane and 1,1,2-trichloroethane represent data measured by Kumagai [89-kum]. The isothermal compressibilities calculated from the fits are systematically lower than data from the literature; the average deviations are −5.3 and −3.1%, respectively (not considering the values extrapolated from the fit for 1,1,2-trichloroethane).

Data for only two isotherms, 298.15 K [51-new/wea] and 295.25 [63-and], were available for 1,1,2,2-tetrachloroethane, and therefore the fit is an interpolation between those two sets. It seems, however, probable that the data by Newitt and Weale [51-new/wea] are lower than correct values (see also the discussion for 1,1- and 1,2-dichloroethane above). This conclusion is supported by the observed negative deviation in isothermal compressibility at 298.15 K (−4.5%, Table 5). The isothermal compressibility at $T =$ 295.25 K resulting from the other data set [63-and] is also lower than the value obtained by the interpolation from the literature data.

No data for isothermal compressibility of chloroethene and *cis*-1,2-dichloroethene were found for a comparison. The values of the parameter c_0 (0.123 720 and 0.069 852, respectively) are, however, outside of the usual range (approximately 0.09 to 0.105).

Similarly as with 1,1,2,2-tetrachloroethane, there were data for only two isotherms, 298.15 K [51-new/wea] and 293.15 [96-hah/ulc], available for *trans*-1,2-dichloroethene. No values of isothermal compressibility were found in the literature, but the fit (Table 3) gives a decrease with increasing temperature {β_T(T=293.15 K, P=0.1 MPa) = 1.105 GPa^{-1} and β_T(T=298.15 K, P=0.1 MPa) = 1.051 GPa^{-1}} which is obviously caused by the positive value of the parameter b_1. This result supports the above-mentioned suggestion that the data measured by Newitt and Weale [51-new/wea] are systematically lower than correct values. In light of this observation it should be pointed out that the fit presented for *trans*-1,2-dichloroethene in Table 3 represents the data for the isotherm 293.15 K [96-hah/ulc] (with c_0 and b_0, since the parameter $T_0 = 293.15$ K) and should not be used for other temperatures.

Table 7. Parameters a_i of Smoothing Function 13 or 14 Fitted to Selected Density Values, $\rho[T,P=0.1\ \text{MPa or } P_{Sat}(T)]$, Critical Densities,[a] ρ_c, Critical Temperatures,[a] T_c, Temperature Ranges of Density Data, T_{min} and T_{max}, and RMSD of the Fits

eq	a_0	a_1	a_2	a_3	a_4	ρ_c/kg·m^{-3}	T_c/K	T_{min}/K	T_{max}/K	RMSD/ kg·m^{-3}	ref
					Chloromethane						
13	1.428932	3.029590	−5.814 254	6.198 836	−1.996 627	363.220	416.25	175.44	414.25	0.220	73-trc, 81-trc
					Dichloromethane						
13	3.003681	−2.197633	2.342 686			440.065	510.00	178.03	383.15	0.205	73-trc
					Trichloromethane						
13	3.563393	−3.860512	3.356 362			499.487	536.40	213.15	333.15	0.615	73-trc
					Tetrachloromethane						
13	1.589943	2.519460	−5.823 132	6.967 929	−2.513 594	557.327	556.40	253.15	554.30	0.412	73-trc
					Bromomethane						
13	5.168382	−11.93268	15.502 549	−5.993 888		620.516	464.00	183.15	333.15	0.099	80-trc
					Dibromomethane						
14	2937.4967	22.587611	−80.387 47	7.313 685			−	273.15	363.15	0.144	80-trc
					Tribromomethane						
14	3559.5341	−196.2118	−10.871 22				−	283.15	403.15	0.023	80-trc
					Iodomethane						
14	3059.7660	−245.5271	−6.939 507					253.15	313.15	0.328	78-kum/iwa
					Chloroethane						
13	2.016815	5.170037	−16.963 62	20.467 362	−7.841 507	324.193	460.40	173.15	453.15	0.402	81-trc
					1,1-Dichloroethane						
13	2.817728	−2.417548	2.409 059			419.319	523.00	263.15	398.15	0.886	73-trc, 85-kum/tak
					1,2-Dichloroethane						
13	2.776599	−2.337741	2.315 300			439.820	561.60	263.15	398.15	0.709	73-trc, 85-kum/tak
					1,1,1-Trichloroethane						
13	3.867403	−5.087538	4.132 311			468.085	545.00	263.15	333.15	0.110	73-trc
13	2.430417	−1.468497	1.797 797			468.085	545.00	298.15	398.15	0.071	89-kum
					1,1,2-Trichloroethane						
13	62.090616	−403.3072	991.090 61	−1053.336	411.253 78	453.756	528.00	263.15	393.15	0.198	73-trc
13	5.561980	−7.606215	5.289 297			453.756	528.00	298.15	398.15	0.307	89-kum
					1,1,2,2-Tetrachloroethane						
13	4.321795	−5.357449	4.186 119			496.595	626.00	263.15	383.15	0.206	73-trc
					Chloroethene						
13	1.308016	1.220248				369.815	429.70	280.99	337.25	0.182	82-cul/ely
					cis-1,2-Dichloroethene						
14	1288.01							293.15	293.15		96-hah/ulc
					trans-1,2-Dichloroethene						
14	1256.79							293.15	293.15		96-hah/ulc
					Trichloroethene						
13	1.306307	1.335124				513.236	571.00	291.25	315.45	0.111	90-fra/com
					Tetrachloroethene						
13	11.632215	−24.97215	16.573 557			571.839	620.20	297.15	315.35	0.427	91-com/fra
					Bromoethane						
13	1.505155	1.350631				506.818	503.90	253.15	313.15	0.868	78-kum/iwa
					1,2-Dibromoethane						
13	2.473417	0.585320				654.571	583.00	293.15	323.15	0.487	49-lag/mcm
					1-Chloropropane						
13	4.152718	−5.739544	4.744 309			309.218	503.00	253.15	343.15	0.129	81-trc
					1-Bromopropane						
13	1.658346	1.175362				455.529	536.00	280.00	340.00	0.112	78-gus/bai
					2-Bromopropane						
13	1.558242	1.126040				462.379	521.00	280.00	320.00	0.406	78-gus/bai
					1-Iodopropane						
14	2223.2254	−138.8672	−7.969 853					287.65	360.65	3.310	43-vog
					1-Chlorobutane						
13	0.266366	4.721455	−2.363 381			303.503	536.00	263.15	363.15	0.189	81-trc
					1-Bromobutane						
13	1.595251	1.237459				421.599	572.00	293.15	323.15	0.041	49-lag/mcm
					1-Bromopentane						
14	1602.0936	−130.4864						283.00	363.00	0.075	77-gus/bai

Table 7. (Continued)

eq	a_0	a_1	a_2	a_3	a_4	ρ_c/kg·m^{-3}	T_c/K	T_{min}/K	T_{max}/K	RMSD/ kg·m^{-3}	ref
						Fluorobenzene					
13	3.655374	−4.722411	3.976 088			357.266	560.09	243.15	353.15	0.068	89-abd/akh
						Hexafluorobenzene					
13	1.699144	1.923190	−2.552 777	1.935 103		555.394	516.73	293.15	490.00	0.164	74-hal/tow
13	3.110978	−3.013351	2.967 418			555.394	516.73	298.11	373.18	0.194	81-dym/rob, 82-dym/gle
						Chlorobenzene					
13	0.117137	12.371210	−28.446 42	29.404 828	−10.707 54	365.451	632.40	253.15	630.15	0.046	90-trc
						1,2-Dichlorobenzene					
14	1664.1672	−125.0781	1.063 348					253.15	323.15	0.029	90-trc
						Chlorocyclohexane					
13	2.709054	−2.120496	2.238 656			332.231	636.00	243.15	298.15	0.030	97-jen/wue
						2,4-Dichloro-1-methylbenzene					
14	1503.1969	−81.51786	−2.492 618					293.00	423.00	0.358	91-ver/mel
						Bromobenzene					
13	2.849480	−2.300548	2.313 943			484.599	670.00	298.15	358.15	0.027	39-gib/loe-1
						2,4-Dibromo-1-methylbenzene					
14	2156.3594	−97.94520	−6.004 001					293.00	423.00	0.536	91-ver/mel
						Iodobenzene					
14	2198.9509	−106.7639	−6.232 634					293.00	423.00	0.399	91-ver/mel

[a] From the database in ref [93-cda]. Critical densities are given with three decimal places, since they were calculated from rounded values of critical molar volumes recorded in the database in ref [93-cda].

The fits of isothermal data (T = 298.15 K) for trichloroethene and tetrachloroethene represent the values reported by Newitt and Weale [51-new/wea] that are probably lower than correct values (see the discussion above on 1,1-dichloroethane, 1,2-dichloroethane, 1,1,2,2-tetrachloroethane, *trans*-1,2-dichloroethene). Despite the fact that some interpolations and extrapolations were necessary to get the literature values of isothermal compressibility at T = 298.15 K (Table 5), rather large negative deviations of isothermal compressibility calculated from the fits support the above conclusions concerning the data [51-new/wea].

The data available for bromoethane are not in good mutual agreement. A tentative fit of data [78-kum/iwa, 88-rut] in the full temperature and pressure ranges resulted in the extreme on the $B(T)$ function at T = 355 K, and therefore the final fit is limited up to 333.15 K. Isothermal compressibilities calculated from the fit agree satisfactorily with data from the literature (average deviation 2.6%); the deviations are, however, systematically negative. Values reported by Millet and Jenner [69-mil/jen] are lower than those of the retained data sets; a separate fit resulted in isothermal compressibilities more than 20% lower than values from the literature.

Both data sets available for 1,2-dibromoethane (T = 293.15 K [60-hil/goc]; T = 303.15 K [68-ski/cus]) are probably incorrect. It should be mentioned that the temperature of the experiment [60-hil/goc] is missing in the original paper and was derived from a comparison of the density value at atmospheric pressure with literature data. Isothermal compressibilities calculated from the fit in Table 3 are lower by about 40% than the values from the literature (Table 5). Data reported by Skinner et al. [68-ski/cus] are probably lower than correct values, since negative deviations of data for some other liquids taken from the same source [68-ski/cus] were observed when fitting available data (ethers [97-cib/hne], aromatic hydrocarbons [99-cib/tak], 1-chlorobutane and chlorobenzene below; see Table 4). It is also worth mentioning that the values of adjustable parameters (Table 3) differ significantly from usual values.

An inflection point was observed on the $B(T)$ curve when fitting all data available for 1-chloropropane [33-bri, 88-rut]. After the pressure range was limited up to 100 MPa, a good fit was obtained which yields a reasonable agreement in isothermal compressibilities (average deviation 2.8%).

Good agreement in isothermal compressibilities (average deviation 1.2%) was obtained for 1-bromopropane from the fit of data reported by Guseinov and Bairamov [78-gus/bai]. Similarly as in the case of bromoethane, large negative deviations are observed for the values reported by Jenner and Millet [71-jen/mil]; a tentative fit of data [71-jen/mil] yielded isothermal compressibilities lower by 14% than data from the literature. The only data available for 2-bromopropane were those reported also by Guseinov and Bairamov [78-gus/bai]. Isothermal compressibilities at 293.15 K calculated from the fit agree well (deviation −0.9%) with the value from the literature. It should be mentioned that the values employed for the reference pressure at temperatures higher than the normal boiling points (1-bromopropane, 344.2 K; 2-bromopropane, 332.9 K) were interpolated values (see Appendix 2 and Table 8).

The fits of data of 1-iodopropane, 1-chlorobutane, 1-bromobutane, and 1-chloropentane by Bridgman [33-bri] give reasonable agreement in isothermal compressibilities (see Table 5). The temperature range of the fit for 1-chlorobutane is enlarged by retaining low pressure data [88-rut]. Large negative deviations are observed for rejected data [68-ski/cus] (see also the discussion for 1,2-dibromoethane above). In the case of 1-bromobutane, a very high pressure data set by Bridgman [42-bri] exhibits extremely large negative deviations; isothermal compressibilities derived from data [42-bri] are several tens of a percent lower than the literature values. The cause may issue from the experimental method used that was based on measurements of volume changes of a sealed lead capsule containing the liquid under investigation. Similarly as in the cases of bromoethane and 1-bromopropane, the data reported by Millet and Jenner [69-mil/jen] for 1-bromobutane are systematically lower (see Table 4); a tentative fit of data [69-mil/jen] yielded isothermal compressibilities lower by

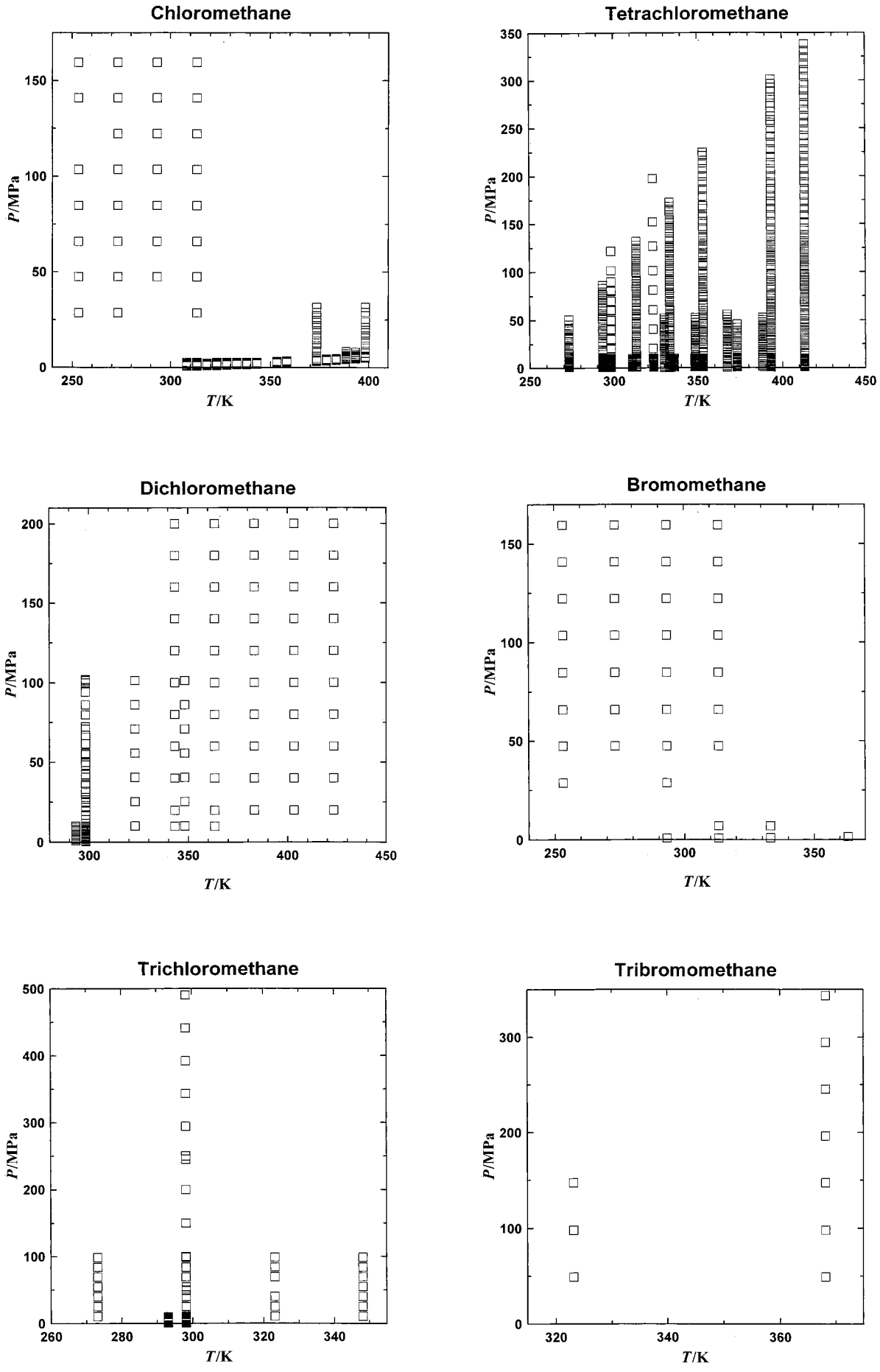
Chloromethane
P/MPa
T/K
Tetrachloromethane
P/MPa
T/K
Dichloromethane
P/MPa
T/K
Bromomethane
P/MPa
T/K
Trichloromethane
P/MPa
T/K
Tribromomethane
P/MPa
T/K

Figure 1.

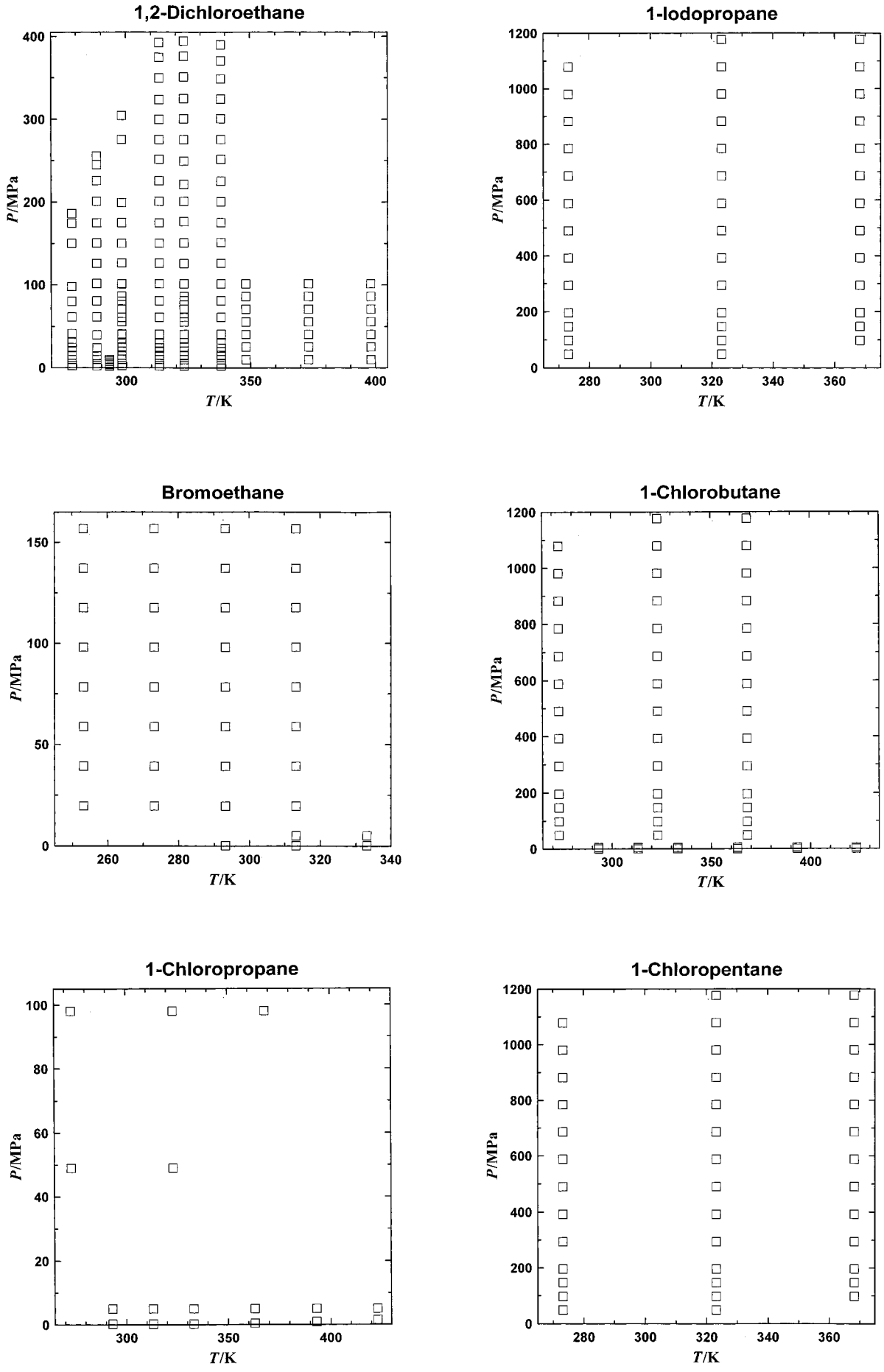

Figure 1. Continued

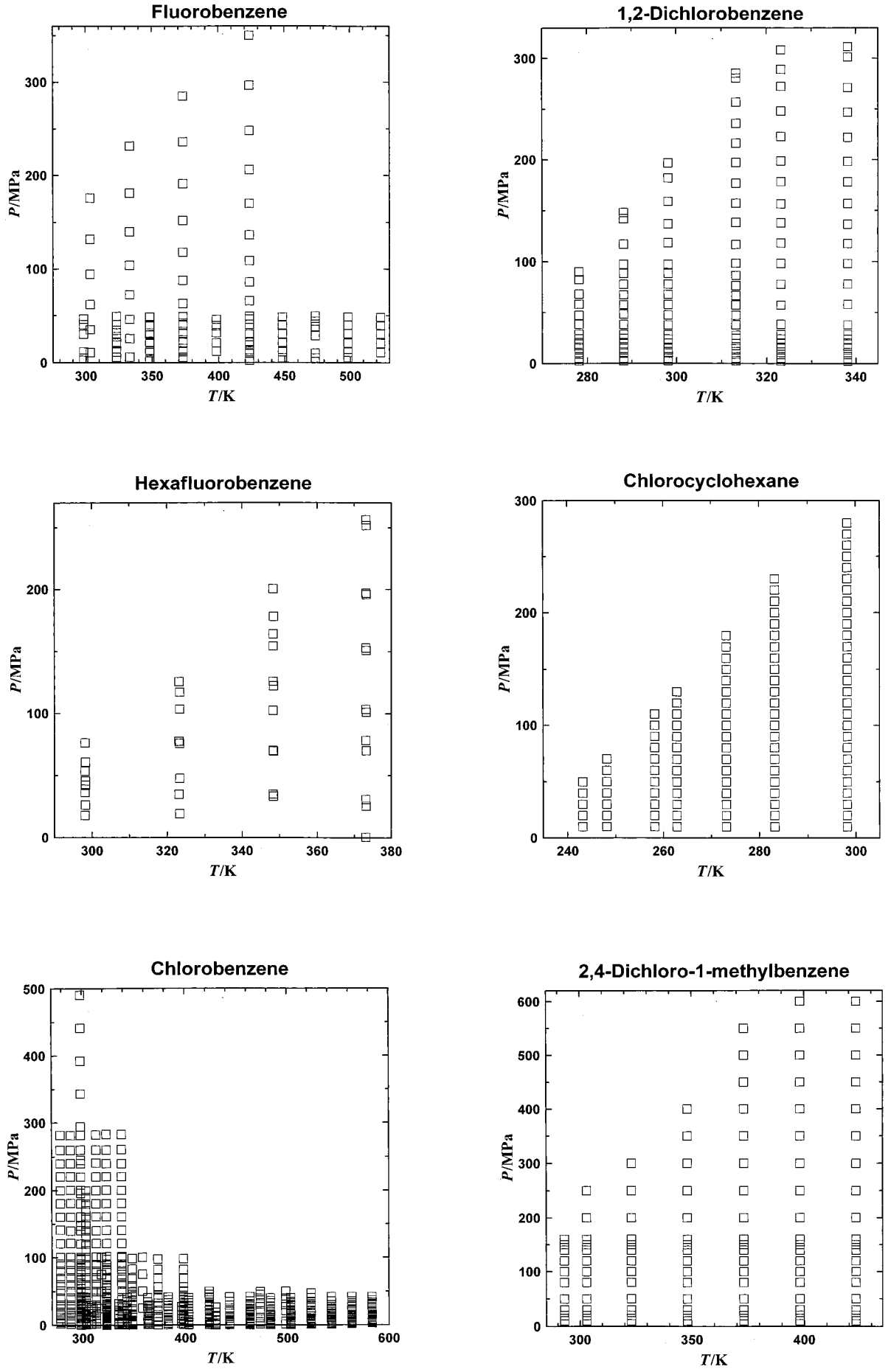

Figure 1. Continued

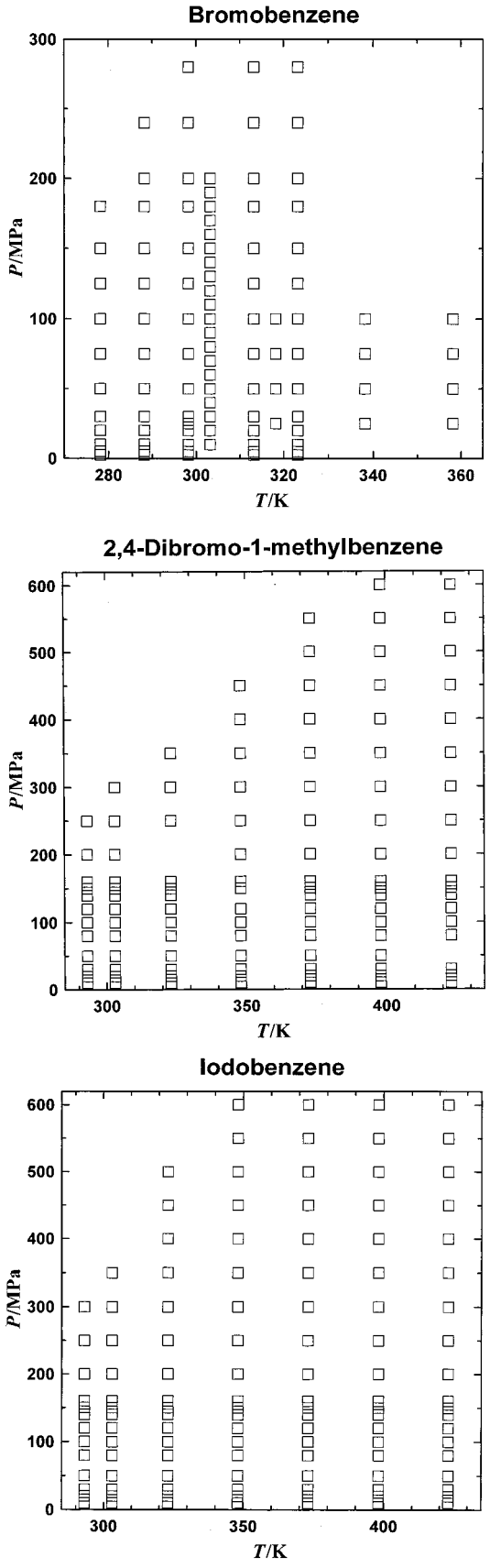

Figure 1. Temperature and pressure coordinates of data points retained in the correlations for the fits in Table 3 where $P-T$ areas of retained data points are not rectangular.

more than 10% than data from the literature. No independent data to evaluate isothermal compressibilities of other liquids measured by Bridgman [33-bri] (1-iodobutane, 1-iodopentane) were found in the literature.

The isothermal compressibility at $T = 293.15$ K evaluated from the fit of the wide temperature data set reported for 1-bromopentane by Guseinov and Bairamov [77-gus/bai] is significantly lower (deviation −15% in an average) than the value from the literature (Table 5). Lower compressibility may be derived from the rejected data set [71-jen/mil] (deviation −22%). A separate fit of data reported by Bridgman [33-bri] resulted in slightly better agreement: $\beta_T(T=293.15\text{ K}, P=0.1\text{ MPa}) = (0.933 \pm 0.007)$ GPa^{-1}. Since one value of isothermal compressibility found in the literature is only available and cannot be confirmed by other data, the parameters (nonzero ones) of this separate fit of Bridgman's data [33-bri] are presented below: $c_0 = 0.096\,759$; $b_0 = 83.1556$ MPa; $b_1 = -60.5845$ MPa·K^{-1}; $b_2 = 25.7875$ MPa·K^{-2}; $T_0 = 323.15$ K; $T_{min} = 273.15$ K; $T_{max} = 368.15$ K; $P_{min} = 49.03$ MPa; $P_{max} = 1176.80$ MPa; RMSD = 0.995 kg·m^{-3}; RMSD$_r$ = 0.068%; bias = −0.018 kg·m^{-3}; $N_p = 38$; $\pm = -8$; $s_w = 0.712$.

The values employed for the reference pressure of 1-bromopentane at temperatures higher than 426.9 K were interpolated values (see Appendix 2 and Table 8).

The fit for fluorobenzene is predominantly based on data reported by Abdullaev et al. [89-abd/akh]; the less accurate data set [74-de /fin] (accuracy of density data declared by the authors is about 3 kg·m^{-3}, which corresponds to the average deviation of these data from the fit, RMSD = 2.45 kg·m^{-3}; see Table 4) is retained to enlarge the pressure range of the fit. The agreement of the calculated isothermal compressibilities with values from the literature is very good (Table 5), even for values extrapolated beyond the temperature range of the fit. Rather large deviations are observed when comparing the compressibilities calculated from the fit with the values evaluated using speed of sound and volumetric data (ρ, α_P) taken from [91-ver/mel]. If these values are excluded, then the average deviation in the temperature range from 303 to 348 K is 1.0%. It is likely that the data [91-ver/mel] are in error, since the thermal expansivity α_P evaluated from densities [91-ver/mel] at atmospheric pressure decreases with increasing temperature. Similarly, the compressed-liquid densities [91-ver/mel] are lower than the data from the other two data sets. Isothermal compressibilities evaluated from a tentative separate fit of data [91-ver/mel] are about 30% lower than data from the literature.

Data of hexafluorobenzene [80-hog/kri] are not in agreement with the values reported by Dymond and co-workers [81-dym/rob, 82-dym/gle]. Besides that, the declared experimental uncertainty of data [80-hog/kri] is large, being about 8 kg·m^{-3}. The final fit represents data of Dymond, and the agreement of isothermal compressibilities calculated from the fit is good; the average deviation is 2.4%, and the deviations are mostly negative.

A rather large number of data sets is available for chlorobenzene. The final fit of retained data (Table 4) yields very good agreement with the values of isothermal compressibility taken from the literature in a large temperature interval from 273.15 to 398.15 K with the average deviation 1.7%.

The fit of one data set available for 1,2-dichlorobenzene yields the deviation of isothermal compressibility from the only available value at $T = 303.15$ K: −3.3%.

The data reported by Jenau and Wuerflinger [97-jen/wue] for chlorocyclohexane cover the temperature range

Table 8. Parameters a_i of Smoothing Function 15, Critical Temperatures,[a] T_c, Critical Pressures, P_c,[a] and Temperature Ranges of Saturated Vapor Pressure Data, T_{min} and T_{max}

a_0	a_1	a_2	a_3	T_c/K	P_c/MPa	T_{min}/K	T_{max}/K	ref
				1-Bromopropane				
−9.689 186	7.167 932	−7.052 820	1.007 272	536.0	4.750	300.0	345.0	56-trc, 77-svo/maj,[b] 84-doh, 93-cda[c]
				2-Bromopropane				
−9.973 169	7.580 876	−6.535 210	−0.809 552 4	521.0	4.920	299.7	331.3	77-svo/maj
				1-Bromopentane				
−8.593 412	3.462 883	−3.066 611	−4.079 971	605.9	3.900[d]	294.1	429.6	56-trc

[a] From the database in ref [93-cda]. [b] Vapor pressures and heats of vaporization. [c] Heat capacities. [d] Estimated by the Lydersen method.

from freezing temperatures up to 298.15 K. The data for T = 228.15 K were rejected due to large deviations (4.5 kg·m^{-3} in an average) that might be caused by the solidification of the substance in the apparatus. The deviations in isothermal compressibilities are positive and rather large (see Table 5), and the extrapolation toward higher temperatures (313.15 K) resulted in the deviation 16%.

No isothermal compressibility data were available for 2,4-dichloro-1-methylbenzene and 2,4-dibromo-1-methylbenzene. The fits represent the data reported by Verveiko et al. [91-ver/mel]. The data for iodobenzene taken from [91-ver/mel] yield a good agreement (1.2% in an average; see Table 5) with the isothermal compressibilities calculated using speed of sound and volumetric data (ρ, α_P) taken from the same source [91-ver/mel], but larger negative deviations are observed when either the volumetric data [49-lag/mcm, 65-mal/hil] along with speed of sound values from [91-ver/mel] or speed of sound and volumetric data [49-lag/mcm] are used. This indicates that isothermal compressibilities calculated from the fit of data [91-ver/mel] might be slightly lower than correct values. Besides that, the values of the parameter c_0 (Table 3) of the fits of data [91-mel/ver] for all these three substances are lower than the usual value (0.09 to 0.105), which signals that the data probably exhibit a systematic error.

Most of the data available for bromobenzene are in good mutual agreement (Table 4). Only one value of isothermal compressibility was available (Table 5); the deviation of the value calculated from the fit is −2.2%.

Malhotra and Woolf [93-mal/woo] proposed a generalized method (group-contribution volume-ratio method; GCVRM) for prediction of the volume ratio $V_r = V(T,P)/V(T,P_{ref}) = \rho(T,P_{ref})/\rho(T,P)$ of chloroalkanes. The method is based on generalized formulas for the Tait parameters C and B (eq 1)

$$C = 0.0912; \quad B/\text{MPa} = -111.677 + 110.089/T_r - 7(N_{Cl} - 3) - 7.7(N_C - 1) \quad (12)$$

where $T_r = T/T_c$ is the reduced temperature and N_{Cl} and N_C are the numbers of chlorine and carbon atoms in a chloroalkane molecule, respectively. Equations 12 are based on selected experimental data for trichloromethane, tetrachloromethane, and 1,1,1-trichloroethane in the reduced temperature range 0.52−0.73 and at pressures up to 150 MPa. Predicted values for various chloroalkanes are compared in Table 6 with experimental data retained for the fits presented in Table 3. In those cases where the maximum experimental pressure significantly exceeds 150 MPa, there are two lines presented in the table; one for the maximum pressure range and the other for pressures limited up to 150 MPa. It is obvious that the GCVRM method yields values that, in average, deviate from the experiment less than 1%. Naturally, the best results are obtained for those three chloroalkanes whose experimental data were employed by Malhotra and Woolf to derive eq 12. Larger deviations are observed for chloromethane and dichloromethane. Here large deviations are observed in the high reduced temperature ranges (greater than 5% for $T_r > 0.90$ in the case of chloromethane, T_c = 416.3 K; greater than 2% for $T_r > 0.79$ in the case of dichloromethane, T_c = 510.0 K), which indicates that a simple reciprocal temperature dependence of the parameter B (eq 12) is not sufficient. The method is not capable of distinguishing between isomers (see the results for 1,1,1-trichloroethane and 1,1,2-trichloroethane in Table 6). On the other hand, the data of both isomers of dichloroethane are represented satisfactorily by the GCVRM method, which yields the "average" values between those two isomers (positive deviations are observed for 1,1-dichloroethane while negative ones are observed for 1,2-dichloroethane).

Acknowledgment

Thanks are expressed to Dr. M. Frenkel and Dr. R. C. Wilhoit (Thermodynamics Research Center, A & M University, College Station, TX) for extracting some speed-of-sound data from the TRC Source Database and to Dr. V. Diky (Research Institute of Physical and Chemical Problems, Minsk, Belorussia) for the help in obtaining papers published in countries of the former Soviet Union.

Appendix 1. Representation of Reference Density Data, $\rho[T,P_{ref}(T)] = \rho(T)$

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

$$\rho(T/\text{K})/(\text{kg·m}^{-3}) = \rho_c\{1 + \sum_{i=0}^{5} a_i(1 - T_r)^{(i+1)/3}\}, \quad T_r = T/T_c \quad (13)$$

$$\rho(T/\text{K})/(\text{kg·m}^{-3}) = \sum_{i=0}^{2} a_i(T/100)^i \quad (14)$$

The values of adjustable parameters a_i obtained by fitting to selected data using a weighted least-squares method are recorded in Table 7 along with some characteristics of the fits. The statistical weights of density values taken from *Thermodynamics Research Center Thermodynamic Tables—Non-Hydrocarbons* (TRC Tables) were related to the number of significant digits presented in the TRC Tables; in other cases the weights were estimated from information in original papers or related to average deviations of the extrapolations. The absence of extremes and inflection points on the function $\rho(T)$ was checked for all fits. Equation 13 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 data, particularly in the region between T_{max} and T_c. Therefore, the fits by eq 13 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 get 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 7, since 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. The only exception is the data set [87-lai/mil] for tetrachloromethane, where the values calculated from function 13 were used.

The results in Table 7 are either (i) the fits of recommended values available in the TRC Thermodynamic Tables combined in several cases with data either presented by authors of density data at elevated pressures or obtained by the extrapolation to the reference pressure 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 references presenting the results of measurements at atmospheric or saturation pressure in wider temperature ranges. With the exception of the fits based on values taken from TRC Tables, the other fits in Table 7 are not the results of a critical evaluation. 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.

The density data for chloroethane required five adjustable parameters for the fit by eq 13; the inflection point appeared, however, at $T = 419$ K. Temperature ranges of data available in the TRC Tables [73-trc] for 1,1-dichloroethane (263.15−313.15 K) and 1,2-dichloroethane (263.15−323.15 K) were extended by retaining the values from [85-kum/tak] at higher temperatures (348.15−398.15 K and 298.15−398.15 K, respectively). Data from the two sources are not in good agreement (better for 1,2-dichloroethane), and thus the fits by eq 13 with more than three parameters led to inflection points and $a_0 < 0$. Average deviations of data sets (RMSD/(kg·m^{-3})) for the fits presented in Table 7 are as follows. 1,1-dichloroethane: 0.162 [73-trc], 1.598 [85-kum/tak]. 1,2-dichloroethane: 0.416 [73-trc], 1.015 [85-kum/tak].

Two fits are given in Table 7 for 1,1,1-trichloroethane and 1,1,2-trichloroethane, since the data from the sources [73-trc, 85-kum/tak] differ significantly. The values for 1,1,1-trichloroethane from [73-trc] are 12 kg·m^{-3} higher in the overlapping temperature interval; for 1,1,2-trichloroethane the densities [73-trc] are higher than those from [85-kum/tak] at lower temperatures and lower than those at higher temperatures. It should be mentioned that data set [85-kum/tak] comprises values obtained by the authors by extrapolation of compressed-liquid data to saturated vapor pressure.

Single values of density at $T = 293.15$ K (as a_0 of eq 14) are given for *cis*- and *trans*-1,2-dichlorethene. Compressed-liquid data [51-new/wea] for *trans*-1,2-dichlorethene at $T = 298.15$ K are presented as the compression without any value of reference density.

Extrapolated reference densities of bromoethane [88-rut] are not consistent with values from [78-kum/iwa]. The fit by eq 13 represents data from the latter source. No reference values are reported in other sources of compressed-liquid data (see Table 2).

The fit for 1-bromopropane represents experimental values [78-gus/bai]; data obtained by extrapolation of compressed-liquid data ([78-gus/bai] for $T > 340$ K and [88-rut]) were not included. No reference values are reported in [71-mil/jen].

Two fits are presented in Table 7 for hexafluorobenzene. The average deviation (RMSD) of data reported by Dymond [81-dym/rob, 82-dym/gle] from the first fit [74-hal/tow] is 1.01 kg·m^{-3}.

Similarly as with compressed-liquid data of chlorocyclohexane [97-jen/wue], the value at $T = 228.15$ K was rejected due to large positive deviation (solidification of the sample).

The fit for bromobenzene represents data from [39-gib/loe-1]. No reference densities are presented in [87-eas/woo].

Appendix 2. Parameters of the Wagner Function for Saturated Vapor Pressure

Saturated vapor functions for several substances were not found in the literature, and thus the available data were correlated by the Wagner function

$$\ln(P_s/P_c) = \{a_0(1 - T_r) + a_1(1 - T_r)^{1.5} + a_2(1 - T_r)^{2.5} + a_3(1 - T_r)^5\}/T_r \qquad T_r = T/T_c \quad (15)$$

where P_s is saturated vapor pressure and P_c and T_c are critical pressure and critical temperature, respectively. The temperature range of experimental data was below or slightly above the normal boiling point. The reference pressures P_{ref} used in correlations by the Tait equation above the normal boiling point are therefore values interpolated between the low temperature range of data and the critical pressure. Where possible the multiproperty fits [96-ruz/maj] were performed correlating simultaneously saturated vapor pressures, heats of vaporization, and heat capacities of liquid and ideal gas. The parameters of eq 15 and references to the experimental data used are given in Table 8.

Note Added after Publishing

This article was released ASAP on 12/21/00 with the correct layout. It was reposted on the Web on 1/11/01 with the rest of the January/February issue. That posting contained errors in the layout of the equations. The correct version was posted on 1/26/01.

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