Reviews

P−*ρ*−*T* Data of Liquids: Summarization and Evaluation. 5. Aromatic Hydrocarbons

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The published experimental data for 28 aromatic hydrocarbons are summarized and reviewed, and the parameters of the Tait equation are given. 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, $\{1 - V(P)/V(P_{ref})\}$), 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. A comparison of isothermal compressibilities calculated from the Tait equation with available data at $P = 0.1$ MPa from the literature is also presented.

Introduction

The work is a continuation of a systematic summarization and critical evaluation of published $P-\rho-T$ data of organic substances in a liquid state. The data for C, H, O substances, (1-alkanols C_1 to C_{10} [94-cib/zik]) and other C, H, O compounds [97-cib/hne, 97-cib/hne-1]) have been reviewed and evaluated. A review of data for a group of hydrocarbons (*n*-alkanes from C_5 to C_{16}) was also published [96-cib/hne]. In this work the published experimental values of relative density, $\rho(T,P)/\rho(T,P = 0.1$ MPa or $P_{sat.})$ and related quantities of liquids containing an aromatic ring in their molecule compiled from the literature are evaluated. The results can be used to calculate the density of compressed liquid using the reference density $\rho(T,P = 0.1$ MPa or $P_{sat.})$ either selected from the literature or measured for a particular sample.

Sources of Data

The original experimental data (5834 data points) processed were extracted from the 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; i.e., only subcritical liquid density data were taken from the source database. Similarly, as in our previous reviews, values (denoted by a letter F in the "data type" column of Table 2) calculated from smoothing functions presented in the papers (mostly the Tait equation), following as much as possible the information concerning the distribution of experimental points given by authors, were included for

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
benzene	71-43-2	C_6H_6
benzene-d_6 (hexadeuteriobenzene)	1076-43-3	C_6D_6
methylbenzene (toluene)	108-88-3	C_7H_8
ethenylbenzene (vinylbenzene, styrene)	100-42-5	C_8H_8
ethylbenzene	100-41-4	C_8H_{10}
1,2-dimethylbenzene (*o*-xylene)	95-47-6	C_8H_{10}
1,3-dimethylbenzene (*m*-xylene)	108-38-3	C_8H_{10}
1,4-dimethylbenzene (*p*-xylene)	106-42-3	C_8H_{10}
propylbenzene	103-65-1	C_9H_{12}
1-(methylethyl)benzene (isopropylbenzene, cumene)	98-82-8	C_9H_{12}
1,2,4-trimethylbenzene (pseudocumene)	95-63-6	C_9H_{12}
1,3,5-trimethylbenzene (mesitylene)	108-67-8	C_9H_{12}
naphthalene	91-20-3	$C_{10}H_8$
1,2,3,4-tetrahydronaphthalene (tetralin)	119-64-2	$C_{10}H_{12}$
butylbenzene	104-51-8	$C_{10}H_{14}$
1-(methylpropyl)benzene (*sec*-butylbenzene)	135-98-8	$C_{10}H_{14}$
1-methylnaphthalene	90-12-0	$C_{11}H_{10}$
hexylbenzene	1077-16-3	$C_{12}H_{18}$
diphenylmethane	101-81-5	$C_{13}H_{12}$
1,1-diphenylethane	612-00-0	$C_{14}H_{14}$
octylbenzene	2189-60-8	$C_{14}H_{22}$
nonylbenzene	1081-77-2	$C_{15}H_{24}$
1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydrochrysene	1610-22-6	$C_{18}H_{24}$
1,1-diphenylheptane	1530-05-8	$C_{19}H_{24}$
1-phenyl-3-(2-phenylethyl)undecane	7225-70-9	$C_{25}H_{36}$
1-pentadecylnaphthalene	55191-63-4	$C_{25}H_{38}$
(3-octylundecyl)benzene	5637-96-7	$C_{25}H_{44}$
1,1-diphenyltetradecane	55268-63-8	$C_{26}H_{38}$

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

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				Benzene				
31-bri	9	323.15	368.15	49.1	343.3	vb	D	
38-gib/kin	25	298.15	338.15	25.0	125.0	va	F	
49-gla/sag	169	310.93	510.93	0.7	68.9	vl	S	
54-bet/hay	5	298.15	313.15	40.6	101.4	va	D[f]	99.99m[e]
57-wal/ric	2	289.15	305.15	5240.0	12100.0	sw	D	
59-gol/vag	68	293.15	561.95	1.2	51.5	bu	D	
59-gol/vag	80	293.15	553.15	6.1	50.7	bu	S	
60-hil/goc	5	293.15	293.15	6.1	40.5	bu	D	
62-hol/wha	10	298.15	298.15	1.0	10.0	vl	F	>99.9[e]
62-hol/wha	10	298.15	298.15	1.0	10.0	vl	F	>99.9[e]
62-hol/wha	60	298.15	349.03	1.0	10.0	vl	F	>99.9[e]
65-sch/has	8	298.15	298.15	20.0	90.0	vs	F	
70-dic	35	295.00	295.00	1900.0	43200.0	sw	D	>99[d]
72-lys	3	297.15	297.15	118.0	722.0	sw	D	
73-rog/bur	10	298.15	298.15	1.0	10.0	ce	F	
75-bur/ric	16	293.15	298.15	1.0	8.0	ce	F	>99m[d]
75-par/jon	33	303.00	433.00	6.0	454.4	vb	D	
77-geh/len	118	298.15	553.15	1.0	300.0	ia	D[g]	
77-gup/han	24	285.15	363.15	2.8	22.1	vs	D	
78-fig/fuc	13	298.15	324.15	13.7	147.0	vb	D	99.2[e]
78-gou	90	293.55	393.65	5.1	40.1	vl	D	
79-kas/fuk	40	298.15	348.15	6.9	105.1	vl	D	99.8v[d]
80-tak	1	298.15	298.15	55.3	55.3	ul	C	>99.0v[e]
81-dym/rob	24	298.38	373.17	16.5	402.2	nd	S	
81-tak	9	303.15	303.15	10.0	90.0	ul	C	
82-dym/gle	4	298.09	373.16	0.4	33.2	mo	D	99.5m[d]
82-dym/gle	23	298.09	373.16	42.6	391.4	vb	D	99.5m[d]
82-tak/ter	24	293.15	313.15	5.0	90.0	ul	C	
82-tak/ter-1	9	303.15	303.15	10.0	90.0	ul	C	
83-kas/fuk	38	298.15	398.15	0.2	97.8	cl	D	99.7m[d]
84-kra/nie	148	322.45	560.69	1.9	59.7	ia	D[g]	
84-mat/van	42	288.15	313.15	2.5	35.0	mo	F	
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[g]	>99.7m[e]
87-str/bal	91	423.16	558.20	0.9	34.0	ia	D[g]	99.999[e]
87-sun/kor	81	283.14	323.13	10.0	170.0	ul	C[g]	>99.5v[d]
88-sid/tej	21	298.20	338.20	0.7	34.5	mo	D	>99m[d]
90-bru/wei	47	293.15	338.15	3.2	130.0	vb	F	
91-chy/gre	19	298.15	318.15	0.6	5.2	vl	D	>99.9w[d]
91-deu/ros	80	298.85	523.15	1.0	300.0	vb	D	
92-lag/bon	23	288.15	323.15	10.0	40.0	mo[i]	D	
92-lag/bon	23	288.15	323.15	10.0	40.0	mo[i]	D	
93-mal/woo	86	298.15	348.15	2.6	278.6	vb	D	
total	1631	283.14	561.95	0.2	43200.0			
				Benzene-d_6				
81-dym/rob	24	298.33	373.22	21.0	400.8	nd	S	
82-dym/gle	7	323.48	373.53	0.4	31.4	mo	D	99.6m[e]
82-dym/gle	25	323.48	373.53	51.2	403.2	vb	D	99.6m[e]
84-mat/van	42	288.15	313.15	2.5	35.0	mo	F	
total	98	288.15	373.53	0.4	403.2			
				Methylbenzene				
57-wal/ric	2	277.15	288.15	5210.0	12150.0	sw	D	
63-and	16	295.45	295.45	68.5	785.9	va	D	
68-ski/cus	11	303.15	303.15	76.0	484.3	vl	D	
69-mop	39	223.15	298.15	10.2	202.8	vb	D	99.9[e]
70-akh/abd	170	298.15	573.15	0.5	50.4	pi	D	99.98w[e]
77-gup/han	24	273.15	363.15	2.8	22.1	vs	D	
78-gou	90	294.45	392.75	5.1	40.1	vl	D	
79-dic	15	295.00	295.00	510.0	40200.0	sw	D	99[d]
82-kas/has	88	273.15	373.15	12.5	250.0	cl	S	>99.5[d]
84-tak/ter	23	293.15	303.15	20.0	160.0	ul	C	
85-alb/gat	19	298.14	399.81	0.2	20.5	mo	D	
85-eas/woo	15	278.15	298.15	25.0	200.0	vb	S	
85-mur/tra	157	179.02	320.30	10.1	263.4	ul	C[g]	
85-tak/ter	16	303.15	303.15	10.0	160.0	ul	F	>99.6v[e]
88-dym/mal	47	298.15	373.15	4.9	459.0	vb	D	>99m[d]
88-dym/mal	10	348.15	348.15	5.7	454.2	vb	D	>99m[d]
88-sid/tej	21	298.20	338.20	0.7	34.5	mo	D	>99m[d]
88-str/bal	111	348.07	593.18	0.2	36.2	ia	D[g]	99.999[e]
91-chy/gre	16	318.15	333.15	0.4	5.0	vl	D	>99.9w[d]
94-tar/cas	48	223.16	303.14	0.1	105.5	rl	D[h]	>99.5[d]
95-hoc/bur	56	244.53	362.64	2.6	62.5	vb	D	99.96m[e]
96-mag/bru	310	180.00	400.00	0.5	35.1	ia	D[h]	99.974m[e]
96-poe/kir[j]	69	323.00	423.00	3.4	64.8	vs	D	99.8[d]
97-poe/kir[j]	69	323.00	423.00	3.4	64.8	vs	D	99.8[d]
total	1442	179.02	593.18	0.1	40200.0			

Table 2. (Continued)

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				Ethenylbenzene				
49-bri	6	298.15	298.15	49.0	294.2	vs	D	
				Ethylbenzene				
90-zho/lag	32	293.10	353.10	5.0	40.0	mo	D	>99[d]
91-chy/gre	18	318.15	333.15	0.4	5.0	vl	D	>99.9w[d]
93-gar/ban	60	318.15	373.15	1.0	10.0	mo	D[g]	99.5m[e]
total	110	293.10	373.15	0.4	40.0			
				1,2-Dimethylbenzene				
49-bri	4	298.15	298.15	49.0	196.1	vs	D	
68-ski/cus	5	303.15	303.15	35.7	213.6	vl	D	
69-akh/ima	165	298.15	623.15	0.1	50.8	pi	D	99.7w[e]
69-akh/ima	36	473.15	573.15	1.3	50.1	pi	D	99.7w[e]
85-tak/ter	18	303.15	303.15	10.0	180.0	ul	F	>99.6v[e]
93-gar/ban	60	318.15	373.15	1.0	10.0	mo	D[g]	99.6m[e]
94-tar/cas-1	59	298.15	298.15	1.4	107.9	rl	D	98.8[e]
94-tar/cas-1	79	257.30	298.46	0.4	78.1	rl	D	98.8[e]
total	426	257.30	623.15	0.1	213.6			
				1,3-Dimethylbenzene				
49-bri	9	298.15	298.15	49.0	441.3	vs	D	
63-and	2	298.15	298.15	175.0	303.8	va	S	
67-mam/akh	70	298.16	473.17	0.4	19.9	pi	D	99.4w[e]
67-mam/akh-1	48	498.15	598.15	0.7	19.8	pi	D	99.4w[e]
67-mam/akh-1	10	523.22	573.21	1.0	19.7	pi	D	99.4w[e]
81-tak	20	303.15	303.15	10.0	200.0	ul	C	
90-yok/mor	4	298.15	298.15	10.0	40.0	pi	D	99.95m
93-gar/ban	60	318.15	373.15	1.0	10.0	mo	D[g]	99.3m[e]
94-tar/cas	30	226.15	299.23	0.4	0.4	rl	D[h]	>99[d]
94-tar/cas	152	229.95	298.15	0.1	109.6	rl	D[h]	>99[d]
95-cha/lee	39	298.15	348.15	1.0	20.0	mo	D	>99m[d]
96-cha/lee-1	18	333.15	413.15	5.0	30.0	mo	D	99.7[e]
total	462	226.15	598.15	0.1	441.3			
				1,4-Dimethylbenzene				
68-ski/cus	3	303.15	303.15	35.7	71.2	vl	D	
69-akh/ima-1	128	323.15	548.15	0.4	50.5	pi	D	99.78w[e]
69-akh/ima-1	29	548.15	598.15	2.6	50.7	pi	D	99.78w[e]
81-tak	5	303.15	303.15	10.0	50.0	ul	C	
90-yok/mor	40	283.15	298.15	10.0	200.0	pi	D	99.90m[e]
93-gar/ban	60	318.15	373.15	1.0	10.0	mo	D[g]	99.7m[e]
94-cas/tar	10	288.18	303.11	0.4	0.4	rl	D[h]	99.6[e]
94-cas/tar	37	288.21	303.14	0.2	42.9	rl	D[h]	99.6[e]
total	312	283.15	598.15	0.2	200.0			
				Propylbenzene				
91-chy/gre	18	318.15	333.15	0.4	5.0	vl	D	>99.9w[d]
				1-(Methylethyl)benzene				
49-bri	17	298.15	298.15	49.0	3922.7	vs	D	
68-ski/cus	10	303.15	303.15	35.7	498.5	vl	D	
91-chy/gre	18	318.15	333.15	0.4	5.0	vl	D	>99.9w[d]
total	45	298.15	333.15	0.4	3922.7			
				1,2,4-Trimethylbenzene				
78-gou	90	294.65	392.55	5.1	40.1	vl	D	
				1,3,5-Trimethylbenzene				
49-bri	6	298.15	298.15	49.0	294.2	vs	D	
87-eas/woo	22	298.15	313.15	2.5	280.0	vb	F	
90-pol/wei	72	262.00	362.20	5.0	200.0	vb	F	99.0[d]
94-bao/cac	32	238.19	298.16	44.8	44.8	rl	D[h]	
94-bao/cac	219	238.15	298.15	0.4	108.2	rl	D[h]	
total	351	238.15	362.20	0.4	294.2			
				Naphthalene				
38-rus/hot	16	378.71	746.48	20.9	40.0	cl	D	
				1,2,3,4-Tetrahydronaphthalene				
49-bri	6	298.15	298.15	49.0	294.2	vs	D	
88-sid/tej	21	298.20	338.20	0.7	34.5	mo	D	>99m[d]
95-cha/lee	45	298.15	348.15	1.0	30.0	mo	D	99m[d]
96-cha/lee-1	18	333.15	413.15	5.0	30.0	mo	D	99.2[e]
total	90	298.15	413.15	0.7	294.2			
				Butylbenzene				
90-zho/lag	32	293.10	353.10	5.0	40.0	mo	D	>99[d]
91-chy/gre	18	318.15	333.15	0.4	5.0	vl	D	>99.9w[d]
total	50	293.10	353.10	0.4	40.0			

Table 2. (Continued)

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
				1-(Methylpropyl)benzene				
85-mak/kis	18	313.00	453.00	9.8	245.3	nd	D	
				1-Methylnaphthalene				
88-sid/tej	21	298.20	338.20	0.7	34.5	mo	D	>99m[d]
95-yok/ebi	30	333.15	333.15	10.0	300.0	pi	D	99.9m[e]
96-cha/lee	45	298.15	348.15	1.0	30.0	mo	D	98m[d]
97-bay/bon	15	303.15	343.15	20.0	100.0	mo	D	>98[d]
total	111	298.15	348.15	0.7	300.0			
				Hexylbenzene				
90-zho/lag	32	293.10	353.10	5.0	40.0	mo	D	97[d]
				Diphenylmethane				
97-cha/lee	18	333.15	413.15	5.0	30.0	mo	D	99.6[e]
				1,1-Diphenylethane				
59-low/spe	30	310.93	372.04	20.0	340.0	vb	S	
				Octylbenzene				
90-zho/lag	32	293.10	353.10	5.0	40.0	mo	D	>99[d]
				Nonylbenzene				
90-zho/lag	32	293.10	353.10	5.0	40.0	mo	D	97[d]
91-kan/lag	12	313.15	353.15	10.0	40.0	mo	D	>97[d]
total	44	293.10	353.15	5.0	40.0			
				1,2,3,4,4a,7,8,9,10,11,12,12a-Dodecahydrochrysene				
59-low/spe	35	310.93	408.15	20.0	340.0	vb	S	
				1,1-Diphenylheptane				
59-low/spe	38	310.93	408.15	20.0	340.0	vb	S	
				1-Phenyl-3-(2-phenylethyl)undecane				
58-cut/mcm	128	310.95	408.15	34.5	1033.7	vb	S	
				1-Pentadecylnaphthalene				
58-cut/mcm	43	333.15	408.15	34.5	551.3	vb	S	
				(3-Octylundecyl)benzene				
58-cut/mcm	126	310.95	408.15	34.5	964.7	vb	S	
				1,1-Diphenyltetradecane				
59-low/spe	32	310.93	408.15	20.0	340.0	vb	S	

[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; ia, isochoric apparatus; mo, mechanical oscillator method; nd, not described or stated in the reference; pi, piezometer of unspecified type; rl, expansion principle; sw, shock wave method; ul, densities evaluated from speed of ultrasound; 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 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] IPTS-68 declared by the researchers. [h] ITS-90 declared by the researchers. [i] Two methods of calibration of DMA 512 vibrating-tube densimeter reported; the method that corresponds to the data set listed first is declared by the researchers to be superior. [j] These two sources present identical data.

some substances if no direct experimental (D) or smoothed values (S) were available in the papers. The $\rho(T,P)$ values calculated from other properties (C) were also included in the evaluation.

Treatment of Data and Method of Data Evaluation

The procedures of treatment of the data and the critical evaluation were essentially the same as those employed for 1-alkanols, and the details may be found in our previous paper [94-cib/zik]. A brief summarization only 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

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

where

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

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

and T_0 is a parameter with a preselected fixed value for which $C(T_0) = c_0$ and $B(T_0) = b_0$ are valid. The reference values, $\rho(T,P_{ref}(T))$ and $P_{ref}(T)$, were selected in the same way as that used previously; i.e., at temperatures below the normal boiling temperature the densities at atmospheric pressure (P_{ref} = 0.101 325 MPa) were used, while for higher temperatures the values along the saturation curve, i.e., saturated liquid densities and saturated vapor pressures, were employed. Experimental values of densities

Table 3. Parameters c_i, b_i, and T_0 of Equation 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 Normal Boiling Temperature

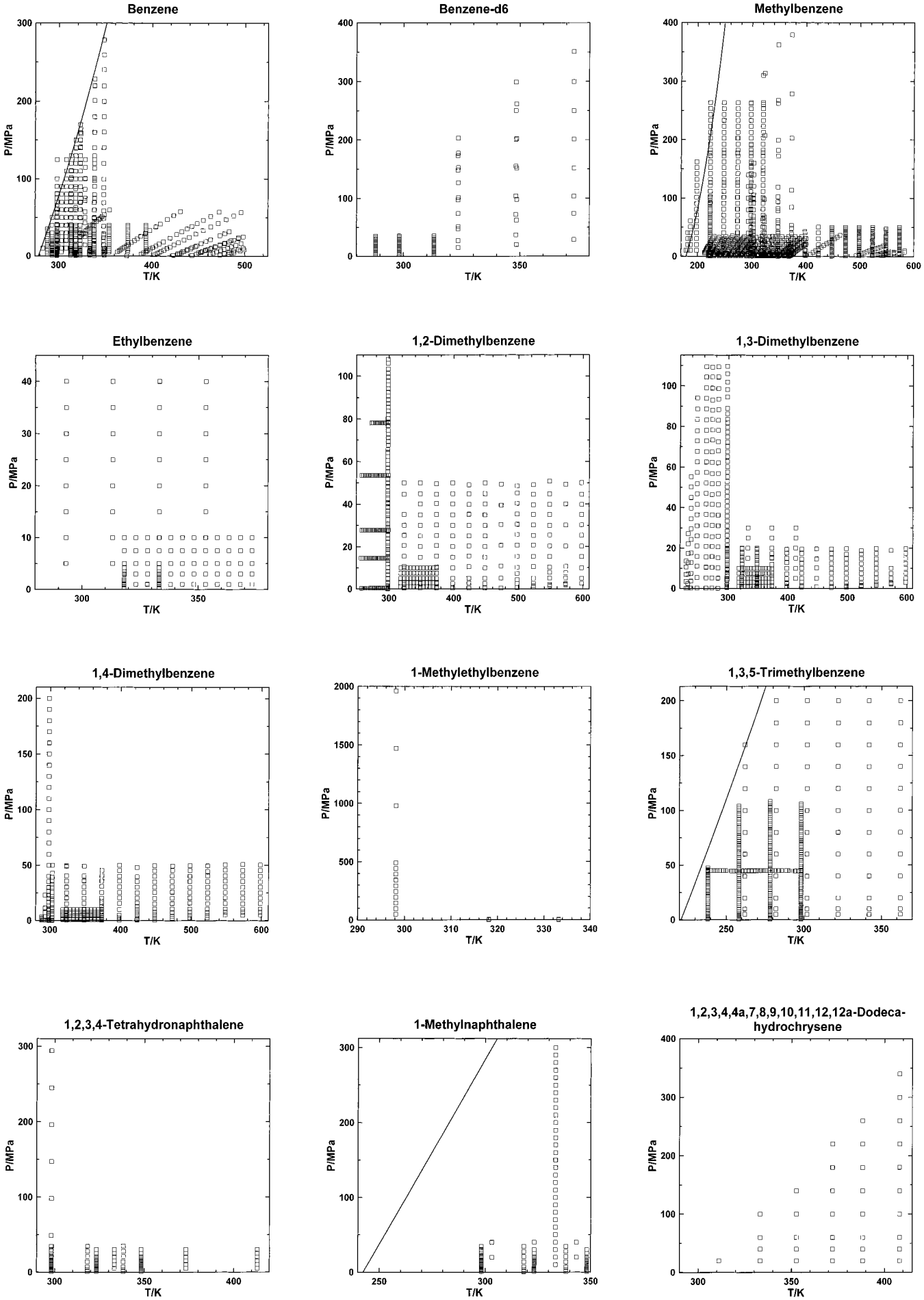
	benzene	benzene-d_6	methyl-benzene	ethenyl-benzene	ethyl-benzene	1,2-dimethyl-benzene	1,3-dimethyl-benzene	1,4-dimethyl-benzene
c_0	0.093 656	0.093 026	0.093 736	0.092 841	0.088 376	0.080 272	0.081 355	0.084 542
c_1/K^{-1}			−0.005004					
b_0/MPa	96.9907	51.3187	104.1019	122.6265	88.9198	99.4733	94.8115	54.0346
b_1/(MPa·K^{-1})	−76.0229	−51.3136	−80.9545		−58.1256	−65.7138	−68.5213	−44.7021
b_2/(MPa·K^{-2})	16.8546	14.9213	22.6002		10.8106	14.2001	19.6299	11.4150
b_3/(MPa·K^{-3})	1.7738		−3.3995			−1.1535	−3.5527	−1.1372
b_4/(MPa·K^{-4})	−1.2453		0.2800				0.3473	
T_0/K	298.15	373.53	298.15	298.15	318.15	298.15	298.15	373.15
T_{min}/K	283.14	288.15	179.02	298.15	293.10	257.30	229.95	288.18
T_{max}/K	499.09	373.22	583.18	298.15	373.15	598.15	598.15	598.15
P_{min}/MPa	0.40	2.50	0.13	49.03	0.40	0.14	0.14	0.17
P_{max}/MPa	278.62	351.00	379.20	294.20	40.00	107.90	109.63	200.00
RMSD/(kg·m^{-3})	0.603	0.807	0.423	0.263	0.189	0.643	0.425	0.523
$RMSD_r$/%	0.079	0.080	0.052	0.027	0.022	0.082	0.054	0.076
bias/(kg·m^{-3})	0.039	0.249	0.061	0.021	0.012	0.187	−0.087	0.021
N_p	718	76	873	6	110	349	386	279
±	−26	36	39	0	32	57	−40	−17
s_w	1.123	0.911	0.927	1.302	0.945	1.033	0.893	0.992
ref($P_{sat.}$)	90-amb/ewi		83-mcg			83-mcg	83-mcg	97-chi/kni

	propyl-benzene	1-(methylethyl)-benzene	1,2,4-trimethyl-benzene	1,3,5-trimethyl-benzene	naphthalene	1,2,3,4-tetrahydro-naphthalene
c_0	0.015 272	0.093 626	0.082 853	0.088 436	0.091 123	0.090 041
b_0/MPa	14.1339	111.1300	103.0400	112.3950	63.4900	151.6228
b_1/(MPa·K^{-1})	−5.5084	−79.5067	−57.5101	−74.5566	−29.0310	−87.0700
b_2/(MPa·K^{-2})			6.7946	7.3889	2.9949	17.3195
T_0/K	318.15	298.15	294.65	298.15	378.71	298.15
T_{min}/K	318.15	298.15	294.65	238.15	378.71	298.15
T_{max}/K	333.15	333.15	392.55	362.20	680.93	413.15
P_{min}/MPa	0.37	0.36	5.10	0.37	20.89	0.69
P_{max}/MPa	5.03	1961.33	40.10	200.00	39.99	294.20
RMSD/(kg·m^{-3})	0.103	0.240	0.397	0.517	3.247	0.196
$RMSD_r$/%	0.012	0.024	0.046	0.056	0.409	0.020
bias/(kg·m^{-3})	−0.008	0.016	0.001	0.185	0.144	0.059
N_p	18	31	90	319	12	90
±	−4	−1	−4	91	2	40
s_w	1.042	0.890	0.913	1.132	1.624	0.939
ref($P_{sat.}$)					90-amb/ewi	

	butyl-benzene	1-(methylpropyl)-benzene	1-methyl-naphthalene	hexyl-benzene	diphenyl-methane	1,1-diphenyl-ethane	octyl-benzene
c_0	0.079 196	0.092 161	0.091 986	0.083 452	0.063 097	0.089 115	0.079 597
b_0/MPa	84.6685	99.2203	152.0557	109.1226	94.8195	154.1532	110.2776
b_1/(MPa·K^{-1})	−53.8613	−62.5075	−90.8224	−52.8623	−56.3975	−75.1358	−74.0081
b_2/(MPa·K^{-2})	19.7739	11.6043	−49.9987		11.6999	8.0478	31.5832
T_0/K	318.15	313.00	333.15	293.10	333.15	310.93	293.10
T_{min}/K	293.10	313.00	298.15	293.10	333.15	310.93	293.10
T_{max}/K	353.10	453.00	348.15	353.10	413.15	372.04	353.10
P_{min}/MPa	0.38	9.80	0.69	5.00	5.00	40.00	5.00
P_{max}/MPa	40.00	245.30	300.00	40.00	30.00	340.00	40.00
RMSD/(kg·m^{-3})	0.133	0.567	0.234	0.279	0.064	0.182	0.141
$RMSD_r$/%	0.016	0.068	0.023	0.032	0.007	0.018	0.017
bias/(kg·m^{-3})	−0.014	0.040	0.046	−0.002	−0.003	0.021	0.001
N_p	49	17	102	32	18	27	32
±	9	1	16	−6	−6	3	0
s_w	0.758	1.013	0.835	0.934	0.909	0.126	0.873

	nonyl-benzene	DHCH[b]	1,1-diphenyl-heptane	1-phenyl-3-(2-phenyl-ethyl)undecane	1-pentadecyl-naphthalene	(3-octylundecyl)-benzene	1,1-diphenyl-tetradecane
c_0	0.084 407	0.085 194	0.086 804	0.093 579	0.088 826	0.090 790	0.086 304
b_0/MPa	121.0218	126.3788	100.5702	104.4649	96.2374	78.6313	102.7318
b_1/(MPa·K^{-1})	−73.6978	−49.1905	−57.0055	−62.0294	−40.9605	−49.0859	−50.8690
b_2/(MPa·K^{-2})	20.9384	28.0661	5.7969	47.4586	20.8847	8.7882	−23.4097
b_3/(MPa·K^{-3})				45.6066			
T_0/K	293.10	408.15	372.04	388.15	408.15	408.15	372.04
T_{min}/K	293.10	310.93	310.93	310.95	333.15	310.95	310.93
T_{max}/K	353.15	408.15	408.15	408.15	408.15	408.15	408.15
P_{min}/MPa	5.00	20.00	20.00	34.46	34.46	34.46	20.00
P_{max}/MPa	40.00	340.00	340.00	1033.65	551.28	964.74	340.00
RMSD/(kg·m^{-3})	0.127	0.270	0.260	0.516	0.292	0.479	0.652
$RMSD_r$/%	0.015	0.026	0.027	0.052	0.031	0.051	0.068
bias/(kg·m^{-3})	0.036	0.008	0.032	0.015	0.025	0.013	0.076
N_p	44	35	37	125	43	115	32
±	8	−5	−1	5	1	−9	4
s_w	0.909	0.185	0.195	0.373	0.223	0.366	0.487

[a] The low limit of pressure ranges is 0.1 MPa or a saturation pressure (whichever is higher) for all fits; P_{min} is the lowest pressure in a particular set of compressed-liquid density data retained for the correlation. [b] DHCH = 1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydrochrysene.


Benzene
Benzene-d6
Methylbenzene
Ethylbenzene
1,2-Dimethylbenzene
1,3-Dimethylbenzene
1,4-Dimethylbenzene
1-Methylethylbenzene
1,3,5-Trimethylbenzene
1,2,3,4-Tetrahydronaphthalene
1-Methylnaphthalene
1,2,3,4,4a,7,8,9,10,11,12,12a-Dodeca-hydrochrysene
P/MPa
T/K

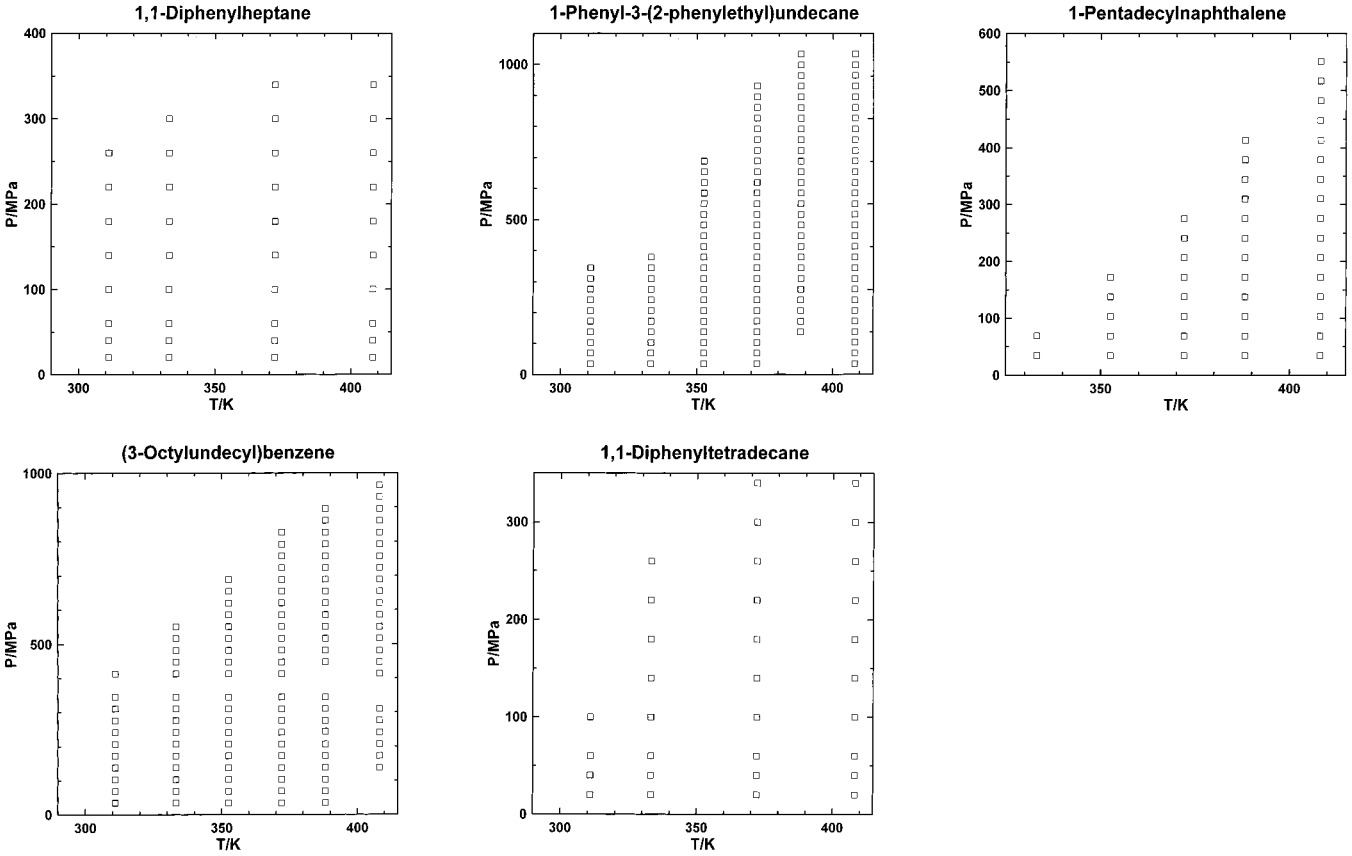


Figure 1. Temperature and pressure coordinates of data points retained in the correlations for the fits in Table 3, where $P-T$ areas of retained data points are not rectangular. The lines represent solid−liquid equilibrium curves: benzene [88-goo], methylbenzene [89-goo], 1,3,5-trimethylbenzene [87-eas/woo], 1-methylnaphthalene [95-yok/ebi].

at atmospheric pressure or at saturation for the same sample reported along with compressed liquid density data were preferably used for the reference density, $\rho(T,P_{ref})$, and thus the values of relative density, $\rho(T,P)/\rho(T,P_{ref} =$ 0.1 MPa or $P_{sat.}$), reported by the authors were correlated by eq 1. In some cases of isothermal data the reference density, $\rho(T,P_{ref})$, was obtained for each isotherm by an extrapolation of experimental compressed liquid density data to 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 the Appendix (Table 6) were employed in the correlations. Saturated vapor pressures were calculated from the smoothing functions taken from the literature (for references see Table 3) and used in the correlations. Selected reference densities, $\rho(T,P_{ref})$ reported in the papers are presented in the form of smoothing functions of temperature in Table 7 in the Appendix.

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

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

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

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

where $\delta\rho_j$ is the experimental uncertainty taken from the source database and either given by the authors (preferably) or estimated by a compiler for the jth density value in a correlated data set, were adjusted by varying the parameter μ_j ($\mu_j = 0$ for rejected values). 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, $\delta\rho_j/\mu_j^{1/2}$, i.e., where the weighted standard deviation of the fit was close to unity. In those cases where only one set of smoothed values (S-type data, Table 2) was available for a particular substance, the statistical weights were not modified ($\mu_j =$ 1 for retained and $\mu_j = 0$ for rejected data points), and therefore the weighted standard deviation, s_w (see below), may differ from unity.

Results

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

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

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

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

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

$$s_\mathrm{w} = [\phi/(N_\mathrm{p} - N_\mathrm{C} - N_\mathrm{B} - 2)]^{1/2} \quad (10)$$

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

Temperature and pressure ranges of the validity of the fits given in the table allow one to avoid extrapolation using eq 1 with the parameters from Table 3 beyond $P-T$ areas of retained data. The $P-T$ areas that are not rectangular are shown in Figure 1, which provides crude information on the distribution of the retained data points. Nonrectangular $P-T$ areas appeared mostly for measurements 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, i.e., 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 for a particular substance (S-type data, see Table 2) was fitted by eq 1, then average deviations of the fit (RMSD, $\mathrm{RMSD_r}$) do not reflect a real accuracy of the experiment and consequently the weighted standard deviation, s_w, is lower than unity (the deviations of smoothed input data from eq 1 are lower than the experimental uncertainty declared by authors).

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.

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 mostly from speed-of-sound measurements and were either taken directly from the papers or calculated from the equation

$$\beta_T = \frac{1}{\rho}\left[\frac{1}{u^2} + \frac{TM\alpha_p^{\,2}}{c_p}\right] \quad (11)$$

where M, u, α_p, and c_p are the molar mass, speed of sound, isobaric thermal expansivity ($\alpha_p = (1/V)(\partial V/\partial T)_p = -(1/\rho)(\partial\rho/\partial T)_p$), and molar isobaric heat capacity, respectively. Values of input quantities in eq 11 were taken from different sources cited in Table 5.

The fit for benzene covers a wide temperature range from 283 to 499 K. Enlargement of the temperature range led to a distortion of the $B(T)$ dependence, and thus the range was limited up to about 60 K below the critical temperature. The final fit, however, exhibits an inflection point of the $B(T)$ function at $T = 498$ K. Several retained data points at low temperatures reported in references 38-gib/kin, 54-bet/hay, and 65-sch/has correspond to undercooled liquid (see Figure 1). Agreement of isothermal compressibilities calculated from the fit (Table 3) with selected independent values (Table 5) is excellent; most deviations are below 1%, and the average deviation in the entire temperature range examined (288−343 K) is 1.4%.

Average deviations among data published for hexadeuteriobenzene are about 0.1%. The fit cannot be improved by adding the b_3-term into $B(T)$ since the inflection point appears at $T = 304$ K. No data on isothermal compressibility were found for a comparison.

The final fit for methylbenzene covers the temperature range 400 K wide. Some data points reported by Muringer et al. [85-mur/tra] at low temperatures correspond to undercooled liquid (see Figure 1). Large negative deviations (over 1 $\mathrm{kg\cdot m^{-3}}$) were observed for isochoric data [88-str/bal] along isochores 717 and 495 $\mathrm{kg\cdot m^{-3}}$; these data points were rejected. The low-temperature limit of the retained data set by Magee and Bruno [96-mag/bru] was set to 213 K since two inflection points appeared on the $B(T)$ function when all data points from this set were retained. The deviations of isothermal compressibilities calculated from the fit from selected experimental values (Table 5) are mostly negative; the agreement is, however, very satisfactory. The average deviation in the entire temperature range examined (180−363 K) is 2.1%.

Compressed-liquid data for ethylbenzene are in good mutual agreement; the average deviations are below 0.03% (Table 4). The deviations between calculated and experimental isothermal compressibilities are positive at lower temperatures and negative at higher temperatures. The average deviation (except for the value extrapolated to 283.15 K, see Table 5) is 1.3%.

Isobaric data ($P = 0.4$ MPa) for 1,3-dimethylbenzene by Taravillo et al. [94-tar/cas] were found to be inconsistent with the reference line $\rho[T,P_\mathrm{ref}(T)]$ [96-trc] (see Table 6 in Appendix) and were rejected, contrary to data for 1,4-dimethylbenzene from the same source. Calculated isothermal compressibilities of all three dimethylbenzenes (xylenes) are in good agreement with experimental values (Table 5) except for compressibility data reported by Kartsev et al. 79-kar/sam where large positive deviations are observed at higher temperatures, particularly for 1,2- and 1,3-dimethylbenzene. Average deviations in the temperature interval from 293.15 to 313.15 K are (not taking into account values from [79-kar/sam]) 0.8%, 0.9%, and 1.5% for 1,2-, 1,3-, and 1,4-dimethylbenzene, respectively.

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]
					Benzene					
31-bri					2.319	0.251	−2.036	7	−7	o
38-gib/kin	298.15	338.15	25.0	125.0	0.158	0.017	−0.049	25	−3	o
49-gla/sag					1.215	0.148	0.616	147	65	o
54-bet/hay	298.15	313.15	40.6	101.4	0.344	0.037	−0.330	5	−5	o
57-wal/ric								0	0	
59-gol/vag					4.216	0.550	−3.089	41	−27	e
59-gol/vag					4.530	0.577	−3.892	48	−48	op
60-hil/goc					1.362	0.153	1.184	5	3	o
62-hol/wha	298.15	298.15	1.0	10.0	0.040	0.005	0.030	10	8	o
62-hol/wha	298.15	298.15	1.0	10.0	0.059	0.007	0.049	10	10	o
62-hol/wha	298.15	349.03	1.0	10.0	0.021	0.002	0.016	60	48	o
65-sch/has	298.15	298.15	20.0	90.0	0.331	0.036	−0.328	8	−8	o
70-dic								0	0	
72-lys					11.756	1.253	−11.756	1	−1	o
73-rog/bur	298.15	298.15	1.0	10.0	0.108	0.012	−0.091	10	−10	o
75-bur/ric	293.15	298.15	1.0	8.0	0.107	0.012	−0.091	16	−16	o
75-par/jon					7.257	0.833	−6.309	25	−25	op
77-geh/len					2.768	0.334	2.004	81	55	e
77-gup/han					1.239	0.139	−0.397	24	−8	p
78-fig/fuc					1.910	0.209	0.970	13	3	ope
78-gou	313.55	393.65	5.1	40.1	0.609	0.073	0.551	75	69	pe
79-kas/fuk					1.066	0.120	−0.685	40	−18	o
80-tak	298.15	298.15	55.3	55.3	0.068	0.007	0.068	1	1	o
81-dym/rob					3.292	0.355	−2.359	20	−18	o
81-tak	303.15	303.15	10.0	90.0	0.234	0.026	−0.216	9	−9	o
82-dym/gle	298.09	373.16	0.4	33.2	0.518	0.060	−0.366	4	−2	oe
82-dym/gle					2.880	0.315	−2.382	19	−19	oe
82-tak/ter	293.15	313.15	5.0	90.0	0.159	0.017	0.090	24	14	o
82-tak/ter-1	303.15	303.15	10.0	90.0	0.234	0.026	−0.216	9	−9	o
83-kas/fuk					1.119	0.129	−0.875	38	−30	o
84-kra/nie	322.45	499.09	1.9	59.7	0.674	0.090	−0.440	100	−68	e
84-mat/van	288.15	313.15	2.5	35.0	0.118	0.013	−0.071	42	−20	o
87-hol/goe	293.15	293.15	2.0	10.0	0.059	0.007	0.049	5	5	o
87-str/bal	423.16	498.19	0.9	31.8	1.955	0.284	1.774	30	30	e
87-sun/kor	283.14	323.13	10.0	170.0	0.468	0.051	−0.397	81	−79	o
88-sid/tej	298.20	338.20	0.7	34.5	0.454	0.053	−0.319	21	−13	o
90-bru/wei	293.15	338.15	3.2	130.0	0.370	0.042	−0.194	45	−27	o
91-chy/gre	298.15	318.15	0.6	5.2	0.093	0.011	−0.025	19	5	o
91-deu/ros					3.605	0.414	−2.365	69	−45	op
92-lag/bon	288.15	323.15	10.0	40.0	0.219	0.025	−0.133	23	−15	o
92-lag/bon					0.522	0.059	0.472	23	23	o
93-mal/woo	298.15	348.15	2.6	278.6	0.668	0.072	0.472	86	68	o
					Benzene-d_6					
81-dym/rob	323.36	373.22	27.0	351.0	1.208	0.120	0.293	20	4	o
82-dym/gle	323.48	348.58	15.0	20.3	1.090	0.118	0.105	2	0	o
82-dym/gle	323.48	348.58	51.2	261.7	1.218	0.120	1.023	12	10	o
84-mat/van	288.15	313.15	2.5	35.0	0.053	0.006	0.013	42	22	o
					Methylbenzene					
57-wal/ric								0	0	
63-and					0.793	0.082	−0.665	9	−9	o
68-ski/cus					14.400	1.499	−13.335	8	−8	o
69-mop	223.15	298.15	10.2	202.8	0.529	0.057	0.331	39	21	o
70-akh/abd	298.15	573.15	0.5	50.4	0.407	0.061	0.160	169	57	p
77-gup/han					0.473	0.056	−0.180	24	−10	p
78-gou					0.896	0.103	0.562	90	54	p
79-dic								0	0	
82-kas/has					1.430	0.152	0.767	88	64	o
84-tak/ter	293.15	303.15	20.0	160.0	0.358	0.039	0.149	23	9	o
85-alb/gat	298.14	399.81	0.2	20.5	0.180	0.023	−0.093	19	−9	p
85-eas/woo					5.460	0.575	0.865	15	5	o
85-mur/tra	179.02	320.30	10.1	263.4	0.093	0.010	0.001	156	−2	o
85-tak/ter					0.645	0.069	−0.432	16	−6	o
88-dym/mal	298.15	373.15	4.9	379.2	1.042	0.111	0.454	44	16	o
88-dym/mal	348.15	348.15	5.7	362.1	1.073	0.111	0.161	9	−3	o
88-sid/tej	298.20	338.20	0.7	34.5	0.156	0.018	−0.062	21	−7	o
88-str/bal	348.07	583.18	0.2	36.2	0.484	0.078	0.074	65	13	e
91-chy/gre	318.15	333.15	0.4	5.0	0.039	0.005	0.033	16	14	o
94-tar/cas	223.16	303.14	0.1	105.5	0.298	0.032	0.181	48	26	p
95-hoc/bur					2.978	0.332	2.397	56	52	p
96-mag/bru	213.00	400.00	0.5	35.0	0.361	0.042	−0.087	264	−96	e
96-poe/kir					1.770	0.216	−0.014	69	−7	p
97-poe/kir					1.770	0.216	−0.014	69	−7	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]
				Ethenylbenzene						
49-bri	298.15	298.15	49.0	294.2	0.263	0.027	0.021	6	0	o
				Ethylbenzene						
90-zho/lag	293.10	353.10	5.0	40.0	0.237	0.027	0.034	32	4	o
91-chy/gre	318.15	333.15	0.4	5.0	0.028	0.003	0.023	18	18	o
93-gar/ban	318.15	373.15	1.0	10.0	0.187	0.023	−0.003	60	10	o
				1,2-Dimethylbenzene						
49-bri					0.773	0.083	0.555	2	2	o
68-ski/cus					3.321	0.363	−2.541	3	−1	o
69-akh/ima	298.15	598.15	0.1	50.8	0.611	0.092	0.140	151	27	p
69-akh/ima					2.042	0.273	1.085	36	6	p
85-tak/ter					1.400	0.153	1.181	10	10	o
93-gar/ban	318.15	373.15	1.0	10.0	0.232	0.028	−0.122	60	−26	o
94-tar/cas-1	298.15	298.15	1.4	107.9	0.288	0.032	−0.163	59	−17	o
94-tar/cas-1	257.30	298.46	0.4	78.1	1.006	0.110	0.773	79	73	e
				1,3-Dimethylbenzene						
49-bri					1.945	0.214	1.854	2	2	o
63-and								0	0	o
67-mam/akh	298.16	473.17	0.5	19.9	0.801	0.100	−0.368	69	−35	p
67-mam/akh-1	498.15	598.15	0.7	19.8	0.312	0.056	0.044	48	14	op
67-mam/akh-1					3.063	0.491	−2.146	10	−6	p
81-tak					1.655	0.183	1.458	10	10	o
90-yok/mor					1.009	0.115	0.932	4	4	o
93-gar/ban	318.15	373.15	1.0	10.0	0.287	0.035	−0.158	60	−22	o
94-tar/cas					3.034	0.335	2.708	30	28	e
94-tar/cas	229.95	298.15	0.1	109.6	0.299	0.033	−0.052	152	−26	p
95-cha/lee	298.15	348.15	1.0	20.0	0.214	0.025	0.124	39	15	o
96-cha/lee-1	333.15	413.15	5.0	30.0	0.175	0.021	0.124	18	14	o
				1,4-Dimethylbenzene						
68-ski/cus					9.044	1.028	−8.784	3	−3	o
69-akh/ima-1	323.15	548.15	0.4	50.5	0.475	0.061	0.133	121	41	pe
69-akh/ima-1	548.15	598.15	5.1	50.7	1.172	0.193	0.040	27	5	e
81-tak	303.15	303.15	10.0	50.0	0.172	0.020	0.132	4	4	o
90-yok/mor	298.15	298.15	10.0	200.0	0.318	0.034	−0.020	20	−6	o
93-gar/ban	318.15	373.15	1.0	10.0	0.233	0.029	−0.153	60	−36	o
94-cas/tar	288.18	303.11	0.4	0.4	0.618	0.072	0.472	10	6	e
94-cas/tar	288.21	303.14	0.2	42.9	0.276	0.032	−0.192	37	−31	p
				Propylbenzene						
91-chy/gre	318.15	333.15	0.4	5.0	0.103	0.012	−0.008	18	−4	o
				1-(Methylethyl)benzene						
49-bri	298.15	298.15	49.0	1961.3	0.368	0.037	0.019	13	−3	o
68-ski/cus					9.979	1.054	−9.811	10	−10	o
91-chy/gre	318.15	333.15	0.4	5.0	0.034	0.004	0.013	18	2	o
				1,2,4-Trimethylbenzene						
78-gou	294.65	392.55	5.1	40.1	0.397	0.046	0.001	90	−4	p
				1,3,5-Trimethylbenzene						
49-bri					1.778	0.192	1.741	4	4	o
87-eas/woo					1.429	0.155	1.226	16	16	o
90-pol/wei	262.00	362.20	5.0	200.0	0.978	0.106	0.590	70	46	o
94-bao/cac	238.19	298.16	44.8	44.8	0.647	0.072	0.625	32	32	e
94-bao/cac	238.15	298.15	0.4	108.2	0.151	0.016	−0.011	217	13	o
				Naphthalene						
38-rus/hot	378.71	680.93	20.9	40.0	3.247	0.409	0.144	12	2	e
				1,2,3,4-Tetrahydronaphthalene						
49-bri	298.15	298.15	49.0	294.2	0.232	0.022	−0.067	6	−2	o
88-sid/tej	298.20	338.20	0.7	34.5	0.222	0.023	−0.115	21	−7	o
95-cha/lee	298.15	348.15	1.0	30.0	0.189	0.020	0.152	45	39	o
96-cha/lee-1	333.15	413.15	5.0	30.0	0.163	0.018	0.072	18	10	o
				Butylbenzene						
90-zho/lag	293.10	353.10	5.0	40.0	0.166	0.020	−0.030	31	−9	o
91-chy/gre	318.15	333.15	0.4	5.0	0.019	0.002	0.015	18	18	o
				1-(Methylpropyl)benzene						
85-mak/kis	313.00	453.00	9.8	245.3	0.567	0.068	0.040	17	1	o
				1-Methylnaphthalene						
88-sid/tej	298.20	338.20	0.7	34.5	0.228	0.023	−0.106	21	−11	o
95-yok/ebi	333.15	333.15	10.0	300.0	0.165	0.016	−0.051	30	−10	o
96-cha/lee	298.15	348.15	1.0	30.0	0.187	0.018	0.117	45	31	o
97-bay/bon	303.15	343.15	20.0	40.0	0.590	0.058	0.527	6	6	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]
				Hexylbenzene						
90-zho/lag	293.10	353.10	5.0	40.0	0.279	0.032	−0.002	32	−6	o
				Diphenylmethane						
97-cha/lee	333.15	413.15	5.0	30.0	0.064	0.007	−0.003	18	−6	o
				1,1-Diphenylethane						
59-low/spe	310.93	372.04	40.0	340.0	0.182	0.018	0.021	27	3	o
				Octylbenzene						
90-zho/lag	293.10	353.10	5.0	40.0	0.141	0.017	0.001	32	0	o
				Nonylbenzene						
90-zho/lag	293.10	353.10	5.0	40.0	0.149	0.018	0.050	32	6	o
91-kan/lag	313.15	353.15	10.0	40.0	0.018	0.002	−0.003	12	2	o
				1,2,3,4,4a,7,8,9,10,11,12,12a-Dodecahydrochrysene						
59-low/spe	310.93	408.15	20.0	340.0	0.270	0.026	0.008	35	−5	o
				1,1-Diphenylheptane						
59-low/spe	310.93	408.15	20.0	340.0	0.260	0.027	0.032	37	−1	o
				1-Phenyl-3-(2-phenylethyl)undecane						
58-cut/mcm	310.95	408.15	34.5	1033.7	0.516	0.052	0.015	125	5	o
				1-Pentadecylnaphthalene						
58-cut/mcm	333.15	408.15	34.5	551.3	0.292	0.031	0.025	43	1	o
				(3-Octylundecyl)benzene						
58-cut/mcm	310.95	408.15	34.5	964.7	0.479	0.051	0.013	115	−9	o
				1,1-Diphenyltetradecane						
59-low/spe	310.93	408.15	20.0	340.0	0.652	0.068	0.076	32	4	o

[a] o, from the same source as the compressed-liquid density data; p, extrapolated to P_{ref} along isotherms using the Tait equation; e, from the smoothing equation (see Appendix, Table 6).

The parameter $B(T)$ of the fit for propylbenzene is a linear function of temperature in the range of experimental $P-\rho-T$ data from 318.15 to 333.15 K (Table 3). The function $B(T)$ has usually a convex shape with negative derivative $dB(T)/dT$, and therefore the extrapolated value $B(T$=298.15K) is likely to be lower than the correct one. This might be a reason the extrapolated value of isothermal compressibility at T = 298.15 K is 16% higher than the experimental value (Table 5). On the other hand, the extrapolated isothermal compressibility calculated from the fit for 1-(methylethyl)benzene (the linear $B(T)$ function) at T = 293.15 K is in much better agreement with experimental values than those calculated for temperatures inside the temperature range of the fit (Table 5). The extrapolation is, however, 5 K only below T_{min} of the fit, compared to 20 K in the case of propylbenzene.

The only $P-\rho-T$ data available in the database for 1,2,4-trimethylbenzene were those reported by Gouel [78-gou] without the values for the reference line. The reference density values $\rho[T,P_{ref}(T)]$ obtained by extrapolation along each isotherm to pressure P_{ref} = 0.101 325 MPa and used in the fit are, on average, lower by 5.4 kg·m^{-3} than smoothed values from 96-trc (see Table 7 in Appendix). The isothermal compressibility calculated from the fit is 3.4% higher than that calculated from speed-of-sound data [44-sch, 52-jac]. The deviation is not caused by an extrapolation since the temperature of the comparison is only 1.5 K lower than T_{min} of the fit.

The $P-\rho-T$ data available for 1,3,5-trimethylbenzene are not in satisfactory agreement; the deviations are as high as 0.2%. The F-type data [90-pol/wei] agree better with the experimental data by Baonza et al. [94-bao/cac] than the values generated from smoothing functions reported by Easteal and Woolf [87-eas/woo]. The final fit given in Table 3 therefore represents experimental data [94-bao/cac] and the smoothed values [90-pol/wei]. The deviations in isothermal compressibilities are, however, rather high (−5.1%, excluding a less accurate value by Shinoda and Hildebrand [61-shi/hil]). The fit of values generated from the smoothing equation reported by Easteal and Woolf [87-eas/woo], which resulted in c_0 = 0.088 773, b_0 = 107.8796 MPa, b_1 = −61.7581 MPa·K^{-1}, T_0 = 298.15 K, T_{min} = 298.15 K, T_{max} = 313.15 K, P_{min} = 2.50 MPa, P_{max} = 280.00 MPa, RMSD = 0.161 kg·m^{-3}, RMSD$_r$ = 0.017%, bias = −0.010 kg·m^{-3}, ± = 0, gives much better agreement in isothermal compressibilities (see Table 5).

The $P-\rho-T$ data set for naphthalene [38-rus/hot] presents compressed-liquid densities for two isobars and therefore the extrapolation along isotherms to obtain reference values $\rho[T,P_{ref}(T)]$ was impossible. The values generated from the smoothing function available in the database [93-cda] were employed instead. The consistency is not good which resulted in rather large average deviation of the fit (RMSD$_r$ = 0.4%).

Data available for 1,2,3,4-tetrahydronaphthalene are in good mutual agreement (see Table 4). The isothermal compressibility calculated from the fit differs from the directly measured value [86-tar/dia] by −0.014 GPa^{-1}, which, due to low compressibility of 1,2,3,4-tetrahydronaphthalene, results in rather large relative deviation (−2.3%).

The fit of data for 1-(methylpropyl)benzene reported by Makhno et al. [85-mak/kis] resulted in satisfactory average deviation (0.07%) after the obviously incorrect density value at T = 373.00 K and P = 245.3 MPa was rejected. The isothermal compressibility calculated from the fit differs significantly (8.1%) from the value calculated using the speed of sound reported in the same source [85-mak/kis].

Data available for 1-methylnaphthalene are in good mutual agreement (see Table 4). The values reported in 97-bay/bon for pressures above 40 MPa were rejected since they were obtained by the authors by an extrapolation of data measured in the range up to 40 MPa. No independent experimental values of isothermal compressibility were found for a comparison.

Data for other substances investigated originated mostly from one source per substance and no isothermal com-

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

	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)
				Benzene					
288.15	0.893 ± 0.002	0.907	−1.5	79-kar/sam[c]	303.15	1.004 ± 0.002	1.010	−0.6	85-tam/mur,[d] 87-tak/ter,[d] 96-trc,[e] 96-zab/ruz[f]
293.15	0.928 ± 0.002	0.933	−0.5	52-jac[c]					
		0.955	−2.8	55-sta/tup[c]			1.011	−0.7	90-sek/ven[c]
		0.978	−5.1	68-day[c]	308.15	1.045 ± 0.002	1.066	−2.0	71-des/bha[c]
		0.917	1.2	71-ric/rog[c]			1.042	0.3	83-dia/lai[c]
		0.929	−0.1	79-kar/sam[c]	313.15	1.088 ± 0.002	1.105	−1.5	55-sta/tup[c]
		0.931	−0.3	85-mar/bha,[d] 96-trc,[e] 96-zab/ruz[f]			1.100	−1.1	79-kar/sam[c]
		0.933	−0.5	85-tam/mur,[d] 87-tak/ter,[d] 96-trc,[e] 96-zab/ruz[f]			1.092	−0.4	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
							1.096	−0.7	87-tak/ter,[d] 96-trc,[e] 96-zab/ruz[f]
298.15	0.965 ± 0.002	0.974	−0.9	71-des/bha[c]	318.15	1.134 ± 0.002	1.139	−0.4	71-des/bha[c]
		0.969	−0.4	78-gro/wil[c]			1.131	0.3	83-dia/lai[c]
		0.963	0.2	83-dia/lai[c]	323.15	1.183 ± 0.002	1.190	−0.6	55-sta/tup[c]
		0.971	−0.6	72-ewi/mar[c]			1.152	2.7	79-kar/sam[c]
		0.970	−0.5	78-kiy/hal,[c] 83-tam/oho,[c] 96-nat[c]			1.191	−0.7	87-tak/ter,[d] 96-trc,[e] 96-zab/ruz[f]
		0.968	−0.3	85-mar/bha,[d] 96-trc,[e] 96-zab/ruz[f]	333.15	1.290 ± 0.003	1.278	0.9	55-sta/tup[c]
		0.971	−0.6	85-tam/mur,[d] 87-tak/ter,[d] 96-trc,[e] 96-zab/ruz[f]			1.285	0.4	79-kar/sam[c]
							1.281	0.7	83-dia/lai[c]
303.15	1.004 ± 0.002	1.028	−2.3	55-sta/tup[c]	343.15	1.410 ± 0.003	1.374	2.6	55-sta/tup[c]
		1.016	−1.2	79-kar/sam[c]			1.433	−1.6	79-kar/sam[c]
		1.009	−0.5	86-kar,[c] 83-nat/tri,[d] 96-trc,[e] 96-zab/ruz[f]					
				Methylbenzene					
180.00	0.420 ± 0.001	0.422	−0.5	91-sun/bom[c]	300.00	0.912 ± 0.002	0.929	−1.8	91-sun/bom[c]
213.86	0.514 ± 0.001	0.527	−2.5	56-mar/sta[c]	303.15	0.933 ± 0.002	0.942	−1.0	74-jai/nor,[d] 96-trc,[e] 96-zab/ruz[f]
200.00	0.472 ± 0.001	0.478	−1.3	91-sun/bom[c]			0.964	−3.4	79-kar/sam[c]
220.00	0.534 ± 0.001	0.542	−1.5	91-sun/bom[c]			0.952	−2.0	83-nat/tri,[d] 85-tam/mur,[d] 96-trc,[e] 96-zab/ruz[f]
232.10	0.576 ± 0.001	0.593	−2.9	56-mar/sta[c]					
240.00	0.606 ± 0.001	0.616	−1.6	91-sun/bom[c]			0.956	−2.4	86-kar[c]
253.91	0.663 ± 0.001	0.687	−3.5	56-mar/sta[c]	308.15	0.968 ± 0.002	0.979	−1.1	71-des/bha[c]
260.00	0.690 ± 0.001	0.703	−1.8	91-sun/bom[c]			0.984	−1.6	71-des/bha,[d] 96-trc,[e] 96-zab/ruz[f]
273.15	0.754 ± 0.001	0.784	−3.8	56-mar/sta[c]			0.975	−0.7	83-dia/lai-1[c]
280.00	0.791 ± 0.001	0.806	−1.9	91-sun/bom[c]			0.977	−0.9	86-gam/tar[c]
283.15	0.809 ± 0.001	0.843	−4.0	79-kar/sam[c]	313.15	1.005 ± 0.002	1.014	−0.9	79-kar/sam[c]
293.15	0.868 ± 0.001	0.884	−1.8	44-sch,[d] 96-trc,[e] 96-zab/ruz[f]			1.025	−1.9	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
		0.899	−3.4	52-jac[c]	318.15	1.043 ± 0.002	1.053	−0.9	83-dia/lai-1,[c] 71-des/bha,[d] 96-trc,[e] 96-zab/ruz[f]
		0.894	−2.9	71-ric/rog[c]					
		0.912	−4.8	79-kar/sam[c]			1.052	−0.9	86-gam/tar[c]
		0.885	−1.9	85-tam/mur,[d] 96-trc,[e] 96-zab/ruz[f]	320.00	1.058 ± 0.002	1.075	−1.6	91-sun/bom[c]
298.15	0.900 ± 0.002	0.92	−2.2	61-shi/hil[c]	323.15	1.084 ± 0.002	1.092	−0.7	79-kar/sam[c]
		0.917	−1.9	71-des/bha[c]	333.15	1.172 ± 0.002	1.195	−1.9	79-kar/sam[c]
		0.920	−2.2	71-des/bha,[d] 96-trc,[e] 96-zab/ruz[f]			1.178	−0.5	83-dia/lai-1[c]
		0.906	−0.7	83-dia/lai-1[c]			1.186	−1.2	86-gam/tar[c]
		0.908	−0.9	74-jai/nor,[d] 96-trc,[e] 96-zab/ruz[f]	343.15	1.270 ± 0.002	1.286	−1.2	79-kar/sam[c]
		0.918	−2.0	85-tam/mur,[d] 96-trc,[e] 96-zab/ruz[f]	353.15	1.379 ± 0.003	1.381	−0.1	79-kar/sam[c]
		0.914	−1.5	86-gam/tar[c]	363.15	1.502 ± 0.003	1.455	3.2	79-kar/sam[c]
		0.913	−1.4	97-oho/tam[c]					
				Ethylbenzene					
283.15	0.798[g]	0.744	7.3	71-hoe/flo[c]	303.15	0.902 ± 0.009	0.892	1.1	74-jai/nor,[d] 96-trc,[e] 96-zab/ruz[f]
293.15	0.848 ± 0.010	0.825	2.8	52-jac[c]	308.15	0.931 ± 0.009	0.927	0.4	71-hoe/flo[c]
		0.840	1.0	44-sch,[d] 96-trc,[e] 96-zab/ruz[f]	313.15	0.961 ± 0.009	0.968	−0.7	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
298.15	0.874 ± 0.010	0.863	1.3	71-hoe/flo[c]	318.15	0.993 ± 0.010	0.997	−0.4	89-mat/aic,[c] 89-mat/tar[c]
		0.859	1.7	74-jai/nor,[d] 96-trc,[e] 96-zab/ruz[f]	333.15	1.097 ± 0.010	1.108	−1.0	71-hoe/flo[c]
		0.868	0.7	89-mat/aic,[c] 89-mat/tar[c]					
		0.868	0.7	95-fuj/tam,[d] 96-trc,[e] 96-zab/ruz[f]					
				1,2-Dimethylbenzene					
283.15	0.731 ± 0.004	0.738	−0.9	79-kar/sam[c]	313.15	0.892 ± 0.004	0.900	−0.9	79-kar/sam[c]
293.15	0.780 ± 0.004	0.781	−0.1	52-jac,[d] 96-trc,[e] 96-zab/ruz[f]			0.889	0.3	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
		0.787	−0.9	79-kar/sam[c]	323.15	0.955 ± 0.004	0.947	0.8	79-kar/sam[c]
		0.770	1.3	58-par/pan,[d] 96-trc,[e] 96-zab/ruz[f]	333.15	1.026 ± 0.005	1.003	2.3	79-kar/sam[c]
298.15	0.806 ± 0.003	0.799	0.9	86-tar/dia-1,[d] 96-trc,[e] 96-zab/ruz[f]	343.15	1.103 ± 0.005	1.053	4.7	79-kar/sam[c]
303.15	0.833 ± 0.004	0.839	−0.7	79-kar/sam[c]	353.15	1.189 ± 0.006	1.121	6.1	79-kar/sam[c]
					363.15	1.284 ± 0.007	1.200	7.0	79-kar/sam[c]
				1,3-Dimethylbenzene					
283.15	0.770 ± 0.002	0.791	−2.6	79-kar/sam[c]	313.15	0.956 ± 0.004	0.921	3.8	79-kar/sam[c]
293.15	0.827 ± 0.003	0.835	−1.0	44-sch,[d] 52-jac,[d] 96-trc,[e] 96-zab/ruz[f]			0.962	−0.6	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
					323.15	1.030 ± 0.004	1.011	1.9	79-kar/sam[c]
		0.816	1.3	58-par/pan,[d] 96-trc,[e] 96-zab/ruz[f]	333.15	1.112 ± 0.004	1.092	1.8	79-kar/sam[c]
		0.839	−1.4	79-kar/sam[c]	343.15	1.201 ± 0.005	1.158	3.7	79-kar/sam[c]
298.15	0.857 ± 0.003	0.864	−0.8	86-tar/dia-1,[d] 96-trc,[e] 96-zab/ruz[f]	353.15	1.300 ± 0.005	1.244	4.5	79-kar/sam[c]
303.15	0.889 ± 0.003	0.892	−0.3	74-jai/nor,[d] 96-trc,[e] 96-zab/ruz[f]	363.15	1.409 ± 0.006	1.306	7.9	79-kar/sam[c]
		0.877	1.4	79-kar/sam[c]					

Table 5. (Continued)

T/K	β_T/GPa^{-1} eq 1[a]	lit.	$\delta\beta_T$[b]/%	ref(s)	T/K	β_T/GPa^{-1} eq 1[a]	lit.	$\delta\beta_T$[b]/%	ref(s)
				1,4-Dimethylbenzene					
288.15	0.836[g]	0.833	0.4	79-kar/sam[c]	303.15	0.925 ± 0.003	0.920	0.5	79-kar/sam[c]
293.15	0.865 ± 0.003	0.855	1.2	44-sch,[d] 96-trc,[e] 96-zab/ruz[f]			0.918	0.8	82-nat/nar,[d] 96-trc,[e] 96-zab/ruz[f]
		0.856	1.1	52-jac,[d] 96-trc,[e] 96-zab/ruz[f]			0.922	0.3	86-kar[c]
		0.842	2.8	58-par/pan,[d] 96-trc,[e] 96-zab/ruz[f]			0.914	1.2	93-sre/nai,[d] 96-trc,[e] 96-zab/ruz[f]
		0.859	0.7	79-kar/sam[c]	308.15	0.957 ± 0.003	0.946	1.3	83-nat/tri,[d] 96-trc,[e] 96-zab/ruz[f]
		0.858	0.8	82-nat/nar,[d] 96-trc,[e] 96-zab/ruz[f]	313.15	0.991 ± 0.003	0.949	4.4	79-kar/sam[c]
		0.848	2.0	85-mar/bha,[d] 96-trc,[e] 96-zab/ruz[f]			0.981	1.0	83-gop/rao,[d] 96-trc,[e] 96-zab/ruz[f]
296.15	0.882 ± 0.003	0.849	4.9	78-pra/pra[c]	323.15	1.064 ± 0.004	1.039	2.4	79-kar/sam[c]
298.15	0.894 ± 0.003	0.91	−1.7	61-shi/hil[c]	333.15	1.144 ± 0.004	1.122	2.0	79-kar/sam[c]
		0.885	1.0	83-nat/tri,[d] 86-tar/dia-1,[d] 96-trc,[e] 96-zab/ruz[f]	343.15	1.232 ± 0.005	1.208	2.0	79-kar/sam[c]
					353.15	1.331 ± 0.005	1.309	1.7	79-kar/sam[c]
		0.876	2.1	85-mar/bha,[d] 96-trc,[e] 96-zab/ruz[f]	363.15	1.440 ± 0.006	1.410	2.1	79-kar/sam[c]
				Propylbenzene					
298.15	0.996[g]	0.857	16.2	95-fuj/tam,[d] 96-trc,[e] 96-zab/ruz[f]					
				1-(Methylethyl)benzene					
293.15	0.813[g]	0.827	−1.7	44-sch,[d] 96-trc,[e] 96-zab/ruz[f]	298.15	0.842 ± 0.003	0.874	−3.7	87-rat/sin,[d] 96-trc,[e] 96-zab/ruz[f]
		0.816	−0.4	52-jac,[d] 96-trc,[e] 96-zab/ruz[f]			0.870	−3.2	95-fuj/tam,[d] 96-trc,[e] 96-zab/ruz[f]
					303.15	0.873 ± 0.009	0.928	−5.9	87-rat/sin,[d] 96-trc,[e] 96-zab/ruz[f]
				1,2,4-Trimethylbenzene					
293.15	0.797[g]	0.771	3.4	44-sch,[d] 52-jac,[d] 96-trc,[e] 96-zab/ruz[f]					
				1,3,5-Trimethylbenzene					
293.15	0.761 ± 0.003	0.803	−5.2	52-jac,[d] 96-trc,[e] 96-zab/ruz[f]	293.15	0.799[g,h]	0.803	−0.5	52-jac,[d] 96-trc,[e] 96-zab/ruz[f]
298.15	0.786 ± 0.003	0.87	−9.7	61-shi/hil[c]	298.15	0.822 ± 0.004[h]	0.828	−0.7	86-tar/dia-1,[d] 96-trc,[e] 96-zab/ruz[f]
		0.828	−5.0	86-tar/dia-1,[d] 96-trc,[e] 96-zab/ruz[f]	303.15	0.846 ± 0.005[h]	0.858	−1.4	86-kar[c]
303.15	0.813 ± 0.004	0.858	−5.2	86-kar[c]					
				1,2,3,4-Tetrahydronaphthalene					
298.15	0.593 ± 0.005	0.607	−2.3	86-tar/dia[c]					
				1-(Methylpropyl)benzene					
313.00	0.93 ± 0.02	0.860	8.1	85-mak/kis,[d] 96-trc-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] [β_T(eq 1) − β_T(lit.)] × 100/β_T(lit.). [c] Isothermal compressibility, $\beta_T = -(1/V)(\partial V/\partial P)_T$. [d] Sound speed. [e] Density and thermal expansivity, $\alpha_p = (1/V)(\partial V/\partial T)_p$. [f] Isobaric heat capacity. [g] Extrapolated beyond the temperature range of the fit. [h] From the fit of F-type values by Easteal and Woolf [87-eas/woo]; see text.

Table 6. Parameters, a_i, of Functions A1 and A3 Used for the Fits in Table 3, Critical Densities,[a] ρ_c, Critical Temperatures,[a] T_c, Temperature Ranges of Validity, T_{min} and T_{max}, Absolute, RMSD, and Relative, RMSD$_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, and References to the Density Data, ref(ρ)

	benzene	methylbenzene	1,2-dimethyl-benzene	1,3-dimethyl-benzene	1,4-dimethyl-benzene	1,3,5-trimethyl-benzene	naphthalene
eq	A1	A1	A1	A1	A1	A1	A3
a_0	1.816 788	2.330 572	1.939 028	1.966 526	2.016 801	12.300 142	1282.372
a_1	−0.144 828	−3.107 839	0.693 214	0.770 424	0.660 504	−32.317 11	0.706 75
a_2	3.651 676	10.483 949	−0.552 518	−0.814 622	−0.770 676	33.770 024	26 417.32
a_3	−5.852 311	−12.816 81	0.742 481	0.944 937	0.997 453	−10.699 35	843.135
a_4	3.501 254	6.294 575					
a_5		−0.2645					
ρ_c[a]/(kg·m^{-3})	301.598	291.585	287.718	282.361	280.126	277.586	
T_c/K	562.16	591.79	630.30	617.05	616.20	637.25	
T_{min}/K	278.70	178.15	247.98	225.31	286.41	238.15	333.00
T_{max}/K	561.15	588.15	628.15	613.15	603.15	353.15	702.00
RMSD/(kg·m^{-3})	0.124	0.227	0.036	0.036	0.031	0.108	0.85
RMSD$_r$/%	0.024	0.041	0.006	0.007	0.005	0.012	0.1
bias/(kg·m^{-3})	−0.005	0.003	−0.001	−0.002	0.000	0.046	
N_p	32	44	41	41	34	53	
±	2	−2	7	3	4	17	
ref(ρ)	96-trc	96-trc	96-trc	96-trc	96-trc	94-bao/cac, 96-trc	93-cda[b]

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

pressibility data (or speed-of-sound and heat capacity data) data were available. Therefore any conclusions concerning their reliability is not possible. The isobar $P = 20$ MPa was rejected for 1,1-diphenylethane due to large negative deviations (3.6−4.6 kg·m^{-3}). The density value for 1,1-diphenylheptane at $T = 310.93$ K and $P = 300$ MPa exhibited the deviation 4.5 kg·m^{-3} and was rejected. The fit for 1-phenyl-3-(2-phenylethyl)undecane required the statistically significant fourth term in the $B(T)$ function (see Table 3), but the inflection point appeared at $T = 354$ K. The data reported for this substance at $T = 388.15$ K and $P < 104$ MPa were rejected due to deviations larger than 1.4 kg·m^{-3}. The isobar $P = 397$ MPa for (3-octylundecyl)-benzene was rejected (deviations from −3.5 to −4.0 kg·m^{-3}) as well as the values at $T = 408.15$ K and for $P < 104$ MPa.

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Table 7. Parameters a_i of Smoothing Functions A1 or A2 Fitted to Reference Density Values ($\rho(T,P_{ref})$), 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
					Benzene-d_6						
A2	1240.1704	−83.895 85	−5.244 859					298.33	373.22	0.032	81-dym/rob 82-dym/gle
					Ethylbenzene[c]						
A2	1068.5906	−52.468 34	−5.640 593					293.10	373.15	0.235	90-zho/lag 91-chy/gre 93-gar/ban
A1	1.873 962	1.207 999	−1.946 025	2.201 250	−0.452 801	283.871	617.24	178.15	616.15	0.164	96-trc
					Propylbenzene						
A1	2.120 703	1.520 552	−3.475 291	3.174 756	−0.285 965	273.170	638.32	173.15	637.15	0.274	96-trc
					1-(Methylethyl)benzene						
A1	1.958 921	0.693 414	−0.839 651	1.080 515		280.829	631.10	177.15	629.15	0.124	96-trc
					1,2,4-Trimethylbenzene						
A2	1181.8435	−127.9835	8.045 603					273.15	353.15	0.013	96-trc
					1,2,3,4-Tetrahydronaphthalene						
A2	1181.3576	−65.549 69	−2.187 500					333.15	413.15	0.000[b]	96-cha/lee-1
					Butylbenzene[d]						
A2	1095.1088	−79.816 09	−0.059 395					293.10	353.10	0.089	90-zho/lag
A2	1082.4276	−70.585 68	−1.784 600					193.15	423.15	0.111	94-trc
					1-(Methylpropyl)benzene[e]						
A2	1062.3953	−59.208 33	−3.273 810					313.00	453.00	0.000[b]	85-mak/kis
A2	1416.6236	−294.6668	35.983 957					273.15	323.15	0.024	96-trc-1
					1-Methylnaphthalene						
A2	1195.7268	−49.511 47	−3.526 464					273.15	423.15	0.133	67-trc
					Hexylbenzene[f]						
A2	1099.4870	−84.393 59	1.190 605					293.10	353.10	0.089	90-zho/lag
A2	1096.1139	−86.585 19	2.087 607					253.15	383.15	0.030	94-trc
					Diphenylmethane						
A2	1213.4399	−63.092 50	−2.500 000					333.15	413.15	0.000[b]	97-cha/lee
					1,1-Diphenylethane						
A2	1226.8121	−77.435 70						310.93	372.04	0.046	59-low/spe
					Octylbenzene[g]						
A2	1081.2117	−80.298 28	1.237 650					293.10	353.10	0.022	90-zho/lag
A2	1054.8852	−63.040 51	−1.557 089					253.15	383.15	0.021	94-trc
					Nonylbenzene[h]						
A2	1076.9383	−77.720 01	0.957 577					293.10	353.15	0.069	90-zho/lag 91-kan/lag
A2	1069.6868	−73.260 14	0.102 162					253.15	323.15	0.026	94-trc
					1,2,3,4,4a,7,8,9,10,11,12,12a-Dodecahydrochrysene						
A2	1213.7306	−50.091 54	−2.085 894					310.93	408.15	0.087	59-low/spe
					1,1-Diphenylheptane						
A2	1171.8673	−78.610 67	1.042 799					310.93	408.15	0.034	59-low/spe
					1-Phenyl-3-(2-phenylethyl)undecane						
A2	1103.7802	−59.675 30	−0.905 630					310.95	408.15	0.104	58-cut/mcm
					1-Pentadecylnaphthalene						
A2	1073.1082	−46.053 64	−2.808 396					333.15	408.15	0.154	58-cut/mcm
					(3-Octylundecyl)benzene						
A2	991.463 65	−31.743 35	−5.041 211					310.95	408.15	0.220	58-cut/mcm
					1,1-Diphenyltetradecane						
A2	1097.8040	−56.953 18	−1.428 472					310.93	408.15	0.133	59-low/spe

[a] From database 93-cda. Critical densities are given with three decimal points since they were calculated from rounded values of critical molar volumes recorded in the database of 93-cda. [b] Polynomial interpolation. [c−h]Average deviations (RMSD) of density data used for the first fit from smoothed TRC values (second fit) in the overlapping temperature ranges are (kg·m^{-3}): 0.44 (*c*), 1.05 (*d*), 1.85 (*e*), 1.32 (*f*), 0.24 (*g*), and 1.87 (*h*).

Appendix

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

$$\rho(T/\mathrm{K})/(\mathrm{kg\cdot m^{-3}}) = \rho_c\{1 + a_0(1 - T_r)^{1/3} + a_1(1 - T_r)^{2/3} + a_2(1 - T_r) + a_3(1 - T_r)^{4/3} + a_4(1 - T_r)^{5/3}\},\quad T_r = T/T_c \quad \text{(A1)}$$

$$\rho(T/\mathrm{K})/(\mathrm{kg\cdot m^{-3}}) = a_0 + a_1(T/100) + a_2(T/100)^2 \quad \text{(A2)}$$

$$\rho(T/\mathrm{K})/(\mathrm{kg\cdot m^{-3}}) = a_0 - a_1T - a_2/(a_3 - T) \quad \text{(A3)}$$

The values of adjustable parameters a_i obtained by fitting to available data using a weighted least-squares method are recorded in Tables 6 and 7 along with some characteristics of the fits. Equation A1 was preferably used in those cases where respective critical parameters (ρ_c, T_c) were available and the data covered a wide temperature range (close to critical temperature). The absence of extremes and inflection points on the function $\rho(T)$ was checked for all fits.

In those cases where the reference density values $\rho(T,P_{ref}(T))$ (see eq 1) were not available (nor original values, nor extrapolated ones), the fits summarized in Table 6 were used for the data sets denoted by letter "e" in the last column of Table 4 to calculate reference density values. The density data retained for the fits in Table 6 were taken from TRC Thermodynamic Tables, except for naphthalene, where the parameters of eq A3 were taken directly from the database [93-cda]. The statistical weights were related to the number of significant digits of density values given in the TRC Tables. The values from TRC Tables were combined with data by Baonza et al. [94-bao/cac] for 1,3,5-trimethylbenzene to enlarge the temperature range of the fit.

Table 7 summarizes the values of adjustable parameters a_i of functions A1 and A2 fitted mostly to the values of experimental densities at atmospheric pressure reported for the same samples as compressed-liquid density data retained in correlations by the Tait equation (see Tables 2−4). The functions were not, unlike the equations summarized in Table 6, employed in smoothing the compressed-liquid density data and are presented as an auxiliary information here, which may be useful particularly for less common substances. The functions can be used to calculate smoothed reference density values for evaluation of compressed liquid densities from eq 1. The fits in Table 7 are not the fits of critically selected experimental data. In several cases the parameters a_i obtained using density values taken from the TRC Thermodynamic Tables are, however, presented. Two fits are given where sufficient data sets were available. No fit for ethenylbenzene (styrene) is presented since the compressed-liquid data are presented as volume ratios at one temperature in the original source [49-bri].

Values by Matsuo and Van Hook [84-mat/van] for hexadeuteriobenzene are not consistent with data reported by Dymond et al. [81-dym/rob, 82-dym/gle] retained for the fit. When all available data were fitted together, the fourth term $a_3(T/100)^3$ in eq A2 became significant, but the inflection point on the $\rho(T)$ function appeared at $T = 317$ K. Average deviations of density values by Chylinski and Gregorowicz [91-chy/gre] for propylbenzene and 1-(methylethyl)benzene (two values per set) from the fits in Table 7 are 0.422 kg·m^{-3} (positive for both data points) and 0.050 kg·m^{-3}, respectively. No original reference density data were available for 1,2,4-trimethylbenzene; the compressed-liquid data are, however, inconsistent with the values from TRC Tables; and densities obtained by extrapolation to P_{ref} of compressed-liquid density data by Gouel [78-gou] are, on average, lower by 5.4 kg·m^{-3} than those from the fit in Table 7. Original reference density values for 1,2,3,4-tetrahydronaphthalene are not in good mutual agreement. The data retained for the fit in Table 7 were those reported for a purified sample with higher purity and of better accuracy declared by authors [96-cha/lee-1]. Similarly, original reference densities for 1-methylnaphthalene fitted together resulted in the fit with RMSD = 2.95 kg·m^{-3}. Data by Chang and Lee [96-cha/lee] for this substance are close to the fit from Table 7 [67-trc] (deviation 0.72 kg·m^{-3} on average); values from other sources (see Table 2) exhibit much larger negative deviations ranging from 1 to 8 kg·m^{-3}.

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