Reviews

$P-\rho-T$ Data of Liquids: Summarization and Evaluation. 4. Higher 1-Alkanols (C_{11}, C_{12}, C_{14}, C_{16}), Secondary, Tertiary, and Branched Alkanols, Cycloalkanols, Alkanediols, Alkanetriols, Ether Alkanols, and Aromatic Hydroxy Derivatives

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The published experimental data for four higher 1-alkanols (C_{11}, C_{12}, C_{14}, C_{16}), secondary, tertiary, and branched alkanols (21 substances), two cycloalkanols, eight polyols, four ether alkanols, and two aromatic hydroxy derivatives (total 41 substances) are summarized and reviewed, and the parameters of the Tait equation are given for 40 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, $\{1 - V(P)/V(P_{ref})\}$), 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 from the literature is also presented.

Introduction

The work is a continuation of a summarization and critical evaluation of published $P-\rho-T$ data of organic substances in a liquid state. The data for two groups of C, H, O substances, 1-alkanols (C_1 to C_{10}, [94-cib/zik]) and other C, H, O compounds except for hydroxy derivatives [97-cib/hne], have been reviewed and evaluated. 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 hydroxy-C, H, O compounds other than (C_1 to C_{10}) 1-alkanols compiled from the literature are evaluated. The results can be used to calculate the density of a compressed liquid using the reference density $\rho(T,P = 0.1$ MPa or $P_{sat})$ selected from the literature or measured for a particular sample.

Sources of Data

The original experimental data (3208 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, supplied by the authors) and summary 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 review [97-cib/hne], also 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 the authors, were included for some substances if no direct experimental (D) or smoothed values (S) were available in the papers. The $P-\rho-T$ values calculated from other properties (C) were also included in the evaluation. A combination F, C given in the "data type" column of Table 2 in a few cases denotes that the $P-\rho-T$ values were evaluated from equations used by authors to smooth the density values calculated from other properties.

Treatment of Data and Method of Data Evaluation

The procedures of treatment of 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

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

where

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

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

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

name (alternative name)	CASRN	formula
1-Alkanols		
1-undecanol	112-42-5	$C_{11}H_{24}O$
1-dodecanol	112-53-8	$C_{12}H_{26}O$
1-tetradecanol	112-72-1	$C_{14}H_{30}O$
1-hexadecanol	36653-82-4	$C_{16}H_{34}O$
Other Alkanols		
2-propanol (isopropyl alcohol)	67-63-0	C_3H_8O
2-butanol (*sec*-butyl alcohol)	78-92-2	$C_4H_{10}O$
2-methyl-1-propanol (isobutyl alcohol)	78-83-1	$C_4H_{10}O$
2-methyl-2-propanol (*tert*-butyl alcohol)	75-65-0	$C_4H_{10}O$
2-pentanol	6032-29-7	$C_5H_{12}O$
3-pentanol	584-02-1	$C_5H_{12}O$
2-methyl-1-butanol	137-32-6	$C_5H_{12}O$
3-methyl-1-butanol (isoamyl alcohol)	123-51-3	$C_5H_{12}O$
2-methyl-2-butanol (*tert*-amyl alcohol)	75-85-4	$C_5H_{12}O$
3-methyl-2-butanol	598-75-4	$C_5H_{12}O$
2-methyl-2-pentanol	590-36-3	$C_6H_{14}O$
4-methyl-2-pentanol	108-11-2	$C_6H_{14}O$
2,2-dimethyl-1-butanol	1185-33-7	$C_6H_{14}O$
2-octanol	123-96-6	$C_8H_{18}O$
3-octanol	589-98-0	$C_8H_{18}O$
3-methyl-1-heptanol	1070-32-2	$C_8H_{18}O$
2-methyl-3-heptanol	18720-62-2	$C_8H_{18}O$
5-methyl-3-heptanol	18720-65-5	$C_8H_{18}O$
6-methyl-3-heptanol	18720-66-6	$C_8H_{18}O$
3-methyl-4-heptanol	1838-73-9	$C_8H_{18}O$
2,7-dimethyl-2-octanol	42007-73-8	$C_{10}H_{22}O$
Cycloalkanols		
cyclopentanol	96-41-3	$C_5H_{10}O$
cyclohexanol	108-93-0	$C_6H_{12}O$
Alkanediols, Alkanetriols		
1,2-ethanediol (ethylene glycol)	107-21-1	$C_2H_6O_2$
1,2-propanediol	57-55-6	$C_3H_8O_2$
1,3-propanediol	504-63-2	$C_3H_8O_2$
1,2,3-propanetriol (glycerine)	56-81-5	$C_3H_8O_3$
1,3-butanediol	107-88-0	$C_4H_{10}O_2$
1,4-butanediol	110-63-4	$C_4H_{10}O_2$
1,5-pentanediol	111-29-5	$C_5H_{12}O_2$
2-methyl-2,4-pentanediol (hexylene glycol)	107-41-5	$C_6H_{14}O_2$
Ether Alkanols		
3-oxa-1-butanol (2-methoxyethanol)	109-86-4	$C_3H_8O_2$
3-oxa-1-heptanol (2-butoxyethanol)	111-76-2	$C_6H_{14}O_2$
3-oxa-1,5-pentanediol (diethylene glycol)	111-46-6	$C_4H_{10}O_3$
3,6-dioxa-1-octanol (diethylene glycol monoethyl ether)	111-90-0	$C_6H_{14}O_3$
Aromatic Hydroxy Derivatives		
3-methyl-1-hydroxybenzene (*m*-cresol)	108-39-4	C_7H_8O
4-allyl-2-methoxy-1-hydroxybenzene (eugenol)	97-53-0	$C_{10}H_{12}O_2$

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

ref	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	meth[a]	data type[b]	sample purity[c]/%
1-Undecanol								
90-naz/sha	75	308.15	598.15	5.0	50.0	pi	D	99.9[d]
1-Dodecanol								
89-mat/mak	21	323.15	348.15	0.9	40.0	mo	D	99[d]
90-naz/sha	74	298.15	598.15	5.0	50.0	pi	D	99.8[d]
93-gar/ban	50	323.15	373.15	1.0	10.0	mo	D[f]	>99.5m[d]
total	145	298.15	598.15	0.9	50.0			
1-Tetradecanol								
89-mat/mak	22	323.15	348.15	0.6	39.7	mo	D	99[d]
1-Hexadecanol								
89-mat/mak	10	348.15	348.15	0.3	40.1	mo	D	99[d]
2-Propanol (Isopropyl Alcohol)								
31-bri	39	273.15	368.15	49.0	1176.8	vb	D	
42-bri	18	298.15	348.15	980.7	4903.3	vs	D	
56-stu	10	303.15	303.15	25.3	202.7	va	D	
56-stu	1	303.15	303.15	101.3	101.3	va	D	
63-gol/bag	82	292.15	504.15	0.3	51.0	bu	D	
63-gol/bag	51	293.15	503.15	2.0	50.7	bu	S	
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
71-tse/sti	58	473.15	493.15	6.9	55.2	ia	S	>99.9[d]
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.9m[d]
77-mor/inu	9	298.15	298.15	10.1	141.9	nd	D	

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]/%
				2-Propanol (Isopropyl Alcohol) (Continued)				
77-mor/mor	1	298.15	298.15	101.3	101.3	va	D	
78-amb/cou	107	385.65	508.15	0.4	10.7	vl	D[f]	99.96m[e]
79-gol/vas	87	292.66	504.30	1.1	49.1	bu	D	
79-zol/gol	22	194.34	273.15	1.1	49.1	bu	D	
80-gol/vas	74	200.00	500.00	1.0	50.0	bu	D	99.84[e]
80-rae/fin	60	298.15	398.15	1.0	411.9	vb	D	
87-kub/tan	40	283.15	348.15	17.8	174.1	cl	D	>99.9w[e]
total	674	194.34	508.15	0.3	4903.3			
				2-Butanol (*sec*-Butyl Alcohol)				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.5m[e]
87-kub/tan	48	283.15	348.15	15.4	206.5	cl	D	>99.9w[e]
92-uos/kit	4	298.15	298.15	50.0	200.0	va	D	
total	66	283.15	348.15	1.0	206.5			
				2-Methyl-1-propanol (Isobutyl Alcohol)				
63-gol/bag	80	294.15	539.95	0.1	52.8	bu	D	
63-gol/bag	75	293.15	533.15	2.0	50.7	bu	S	
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.0m[e]
79-vas/gol	87	297.66	543.75	1.1	49.1	bu	D	99.87[e]
79-zol/gol	7	240.22	241.01	1.1	49.1	bu	D	
80-gol/vas	82	240.00	540.00	1.0	50.0	bu	D	99.84[e]
87-kub/tan	48	283.15	348.15	15.8	206.5	cl	D	>99.9w[e]
total	393	240.00	543.75	0.1	206.5			
				2-Methyl-2-propanol (*tert*-Butyl Alcohol)				
87-kub/tan	21	323.15	348.15	6.7	95.7	cl	D	>99.9w[e]
				2-Pentanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.9m[d]
95-wap/kar	89	234.00	433.00	10.0	200.0	vs	D	>99[d]
total	103	234.00	433.00	1.0	200.0			
				3-Pentanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.5m[e]
95-wap/kar	85	233.60	433.10	10.0	200.0	vs	D	>99[d]
total	99	233.60	433.10	1.0	200.0			
				2-Methyl-1-butanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.5m[e]
				3-Methyl-1-butanol (Isoamyl Alcohol)				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.0m[e]
81-gol/vas	109	273.15	587.37	1.1	49.1	bu	D	96.82[e]
total	123	273.15	587.37	1.0	49.1			
				2-Methyl-2-butanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.5m[e]
				3-Methyl-2-butanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.0m[e]
				2-Methyl-2-pentanol				
76-sah/gag	14	293.15	298.15	1.0	7.0	ce	F, C	99.5m[e]
				4-Methyl-2-pentanol				
92-uos/kit	4	298.15	298.15	50.0	200.0	va	D	
				2,2-Dimethyl-1-butanol				
91-ede/bar	38	258.20	290.00	10.0	130.0	vs	S	99.9[e]
				2-Octanol				
68-joh/dan	23	258.90	363.60	100.0	400.0	vb	F	
				3-Octanol				
33-bri	29	273.15	368.15	49.0	1176.8	vb	D	
68-joh/dan	26	250.90	361.10	100.0	400.0	vb	F	
total	55	250.90	368.15	49.0	1176.8			
				3-Methyl-1-heptanol				
33-bri	35	273.15	368.15	49.0	1176.8	vb	D	
				2-Methyl-3-heptanol				
33-bri	32	273.15	368.15	49.0	1176.8	vb	D	
68-joh/dan	37	216.40	363.50	100.0	400.0	vb	F	
total	69	216.40	368.15	49.0	1176.8			
				5-Methyl-3-heptanol				
68-joh/dan	33	226.80	364.40	100.0	400.0	vb	F	
				6-Methyl-3-heptanol				
33-bri	33	273.15	368.15	49.0	1176.8	vb	D	
				3-Methyl-4-heptanol				
33-bri	34	273.15	368.15	49.0	1176.8	vb	D	

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]/%
				2,7-Dimethyl-2-octanol				
55-kus	40	298.15	353.15	19.6	196.1	nd	D	
				Cyclopentanol				
82-wis/wue	68	273.30	324.90	10.0	230.0	vs	S	99.9[e]
				Cyclohexanol				
90-rie/sch	3	313.20	313.20	10.0	30.0	vs	S	98[d]
				1,2-Ethanediol (Ethylene Glycol)				
32-bri	34	273.15	368.15	49.0	1176.8	vb	D	
41-gib/loe	20	298.15	378.15	25.0	100.0	vl	F	
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
81-dic	13	295.00	295.00	740.0	51400.0	sw	D	98[e]
82-kob/nis	4	298.15	298.15	49.0	196.1	vs	D	
83-nak/miy	1	298.15	298.15	101.3	101.3	va	D	
90-miy/tak	4	298.15	298.15	50.0	200.0	va	D	
90-won/hay	18	298.20	348.20	0.7	6.9	mo	D	99.9[d]
total	95	273.15	378.15	0.7	51400.0			
				1,2-Propanediol				
32-bri	41	273.15	368.15	49.0	1176.8	vb	D	
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
90-miy/tak	4	298.15	298.15	50.0	200.0	va	D	
total	46	273.15	368.15	49.0	1176.8			
				1,3-Propanediol				
32-bri	34	273.15	368.15	49.0	1176.8	vb	D	
83-nak/miy	1	298.15	298.15	101.3	101.3	va	D	
90-miy/tak	8	298.15	298.15	20.0	200.0	va	D	
total	43	273.15	368.15	20.0	1176.8			
				1,2,3-Propanetriol (Glycerine)				
26-bri	6	303.15	303.15	196.1	1176.8	vs	D	
32-bri	41	273.15	368.15	49.0	1176.8	vb	D	
57-wal/ric	2	291.15	303.15	7660.0	17030.0	sw	D	
69-mcd/for	98	223.15	353.15	49.0	274.6	vb	F	99.7a[d]
81-dic	13	295.00	295.00	860.00	56100.0	sw	D	99.5[e]
83-nak/miy	1	298.15	298.15	101.3	101.3	va	D	
90-miy/tak	8	298.15	298.15	20.0	200.0	va	D	
total	169	223.15	368.15	20.0	56100.0			
				1,3-Butanediol				
69-mcd/for	56	233.15	303.15	49.0	274.6	vb	F	
				1,4-Butanediol				
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[e]
				1,5-Pentanediol				
69-mcd/for	45	253.15	308.15	49.0	274.6	vb	F	
				2-Methyl-2,4-pentanediol (Hexylene Glycol)				
69-mcd/for	63	223.15	303.15	49.0	274.6	vb	F	
				3-Oxa-1-butanol (2-Methoxyethanol)				
87-led	52	298.15	343.15	10.0	300.0	vb	S	99.5[d]
				3-Oxa-1-heptanol (2-Butoxyethanol)				
93-mal/woo	138	288.15	348.15	2.6	380.7	vb	D	99.9m[d]
				3-Oxa-1,5-pentanediol (Diethylene Glycol)				
32-bri	34	273.15	368.15	49.0	1176.8	vb	D	
				3,6-Dioxa-1-octanol (Diethylene Glycol Monoethyl Ether)				
77-akh/ima	93	298.15	448.15	0.4	25.2	pi	D	
				3-Methyl-1-hydroxybenzene (*m*-Cresol)				
68-bel/erg	11	288.15	363.15	19.6	78.5	nd	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]
95-ran/lew	160	353.15	503.15	10.0	400.0	ca	C	>99[d]
total	237	288.15	503.15	0.7	400.0			
				4-Allyl-2-methoxy-1-hydroxybenzene (Eugenol)				
32-bri	7	273.15	273.15	49.0	490.3	vb	D	

[a] Method used for measurements: bu, buoyancy method; ca, densities obtained by integration from thermal expansivities measured by the calorimetric method; ce, densities evaluated by integration from isothermal compressibilities obtained by the 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 upspecified type; sw, shock wave method; 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 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; a, mass percent assuming water as an impurity; m, mole percent; w, mass percent. [d] Purity of source material is given only. [e] Final purity of the sample. [f] IPTS-68 declared by the researchers.

and T_0 is a parameter with a preselected fixed value for which $C(T_0) = c_0$ and $B(T_0) = b_0$ hold. The reference values, $\rho(T,P_{ref}(T))$ and $P_{ref}(T)$, were selected in the same way as 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 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. If the reference values were not available in the original source, then densities obtained from the equations summarized in Appendix I were employed in the correlations. In those few cases where the correlations were performed in the temperature region above normal boiling temperature (i.e., where either both the reference density values $\rho(T,P_{ref} = P_{sat})$ and the compressed-liquid density data or relative quantities at temperatures above normal boiling point were available), saturated vapor pressures were calculated from the smoothing functions taken from the literature (see Appendix I) and used in the correlations. Reference densities, $\rho(T,P_{ref})$, reported in the papers are presented in the form of smoothing functions of temperature in Appendix II.

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

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

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 taken into 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

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

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.

Results

Table 3 records the values of the parameters of eq 1 for each substance (except for 1,4-butanediol where only one experimental compressed-liquid data point was available) along with some statistical information of the fits defined as follows:

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

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

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

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

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

where N_p is the overall number of experimental data points retained for the correlation. The characteristics are given in an absolute density scale ($kg\cdot m^{-3}$), which is more illustrative than in a relative density scale. Temperature and pressure ranges of validity of the fits given in the table allow one to avoid extrapolation using eq 1 with the parameters from Table 3 beyond $P-T$ areas of retained data. The $T-P$ areas that are not rectangular are shown in Figure 1, which provides crude information on the distribution of the retained data points. Nonrectangular $T-P$ areas appeared mostly for measurements where the $T-P$ range approached the vicinity of a solid−liquid equilibrium line.

Additional correlations were performed for several substances, mostly in those cases where two contradictory data sets were available. The results (parameters and characteristics) of those fits are given for each particular substance in either the text below or Table 5.

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 $T-P$ areas of the retained data (see Table 3 and Figure 1).

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. Often the values at temperatures above normal boiling temperature were rejected since no reference values, $\rho(T,P_{sat})$, were available. 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.

Similarly as in our previous paper [97-cib/hne], 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 6, which provides a rough

Table 3. Parameters c_i, b_i, and T_0 of Eq 1, Temperature and Pressure Ranges,[a] T_{min}, T_{max}, and P_{min}, and P_{max}, Absolute, RMSD, and Relative, $RMSD_r$, Root Mean Square Deviations, Biases, bias, Number of Data Points, N_p, ±, and Weighted Standard Deviations, s_w

	1-undecanol	1-dodecanol	1-tetradecanol	1-hexadecanol	2-propanol	2-butanol	2-methyl-1-propanol	2-methyl-2-propanol
c_0	0.100151	0.090832	0.095515	0.090779	0.089002	0.089025	0.086562	0.08336
b_0/MPa	108.8233	112.7012	121.6180	102.7420	79.1705	92.9212	72.5122	54.7762
b_1/MPa·K^{-1}	−62.9018	−64.1566	−61.7828		−48.9692	−58.7366	−52.0834	−50.2672
b_2/MPa·K^{-2}	13.5505	9.4975			−4.2479	−6.2402	−4.3429	
b_3/MPa·K^{-3}	−1.3569							
T_0/K	323.15	323.15	323.15	348.15	298.15	298.15	323.15	323.15
T_{min}/K	308.15	298.15	323.15	348.15	273.15	283.15	283.15	323.15
T_{max}/K	598.15	598.15	348.15	348.15	400.00	348.15	376.52	348.15
P_{min}/MPa	5.00	0.85	0.55	0.30	1.00	1.00	1.00	6.70
P_{max}/MPa	50.00	50.00	39.65	40.10	173.90	206.50	206.50	95.70
RMSD/kg·m^{-3}	0.814	0.710	0.091	0.077	0.424	0.526	0.527	0.121
$RMSD_r$/%	0.116	0.100	0.011	0.009	0.054	0.061	0.067	0.015
bias/kg·m^{-3}	−0.098	0.165	−0.003	−0.002	0.098	0.340	0.302	0.009
N_p	75	131	22	10	85	66	117	21
±	−11	31	−2	0	17	42	55	−1
s_w	1.160	1.070	1.010	0.995	0.969	0.935	1.009	1.013

	2-pentanol	3-pentanol	2-methyl-1-butanol	3-methyl-1-butanol	2-methyl-2-butanol	3-methyl-2-butanol	2-methyl-2-pentanol	4-methyl-2-pentanol
c_0	0.099534	0.095181	0.071788	0.069883	0.065996	0.063648	0.060714	0.082676
b_0/MPa	91.5486	111.7756	82.9742	80.0472	65.2033	69.2284	62.4508	85.8117
b_1/MPa·K^{-1}	−63.4627	−74.4979	−43.7423	−10.8179	−58.8448	−57.6943	−49.9541	
b_2/MPa·K^{-2}	13.9496	12.5030		−20.1506				
T_0/K	313.20	283.60	293.15	273.15	293.15	293.15	293.15	298.15
T_{min}/K	234.00	233.60	293.15	273.15	293.15	293.15	293.15	298.15
T_{max}/K	373.40	373.40	298.15	386.90	298.15	298.15	298.15	298.15
P_{min}/MPa	1.00	1.00	1.00	1.00	1.00	1.00	1.00	50.00
P_{max}/MPa	200.00	200.00	7.00	49.14	7.00	7.00	7.00	200.00
RMSD/kg·m^{-3}	0.315	0.268	0.004	0.616	0.003	0.002	0.004	0.250
$RMSD_r$/%	0.037	0.032	0.000	0.079	0.000	0.000	0.001	0.029
bias/kg·m^{-3}	−0.008	0.044	0.001	−0.159	0.000	0.000	0.000	0.004
N_p	70	63	14	35	14	14	14	4
±	−4	−3	2	−3	0	2	−2	2
s_w	1.162	1.096	0.004	0.830	0.004	0.003	0.005	1.031

	2,2-dimethyl-1-butanol	2-octanol	3-octanol	3-methyl-1-heptanol	2-methyl-3-heptanol	5-methyl-3-heptanol	6-methyl-3-heptanol	3-methyl-4-heptanol
c_0	0.066655	0.090457	0.093694	0.094500	0.095988	0.076436	0.092418	0.090744
b_0/MPa	76.8570	114.7054	76.1936	108.1446	85.2795	113.6320	93.1421	92.7699
b_1/MPa·K^{-1}	−30.5164	−72.1325	−43.1838	−58.6203	−14.2752	−64.8075	−57.1193	−63.2003
b_2/MPa·K^{-2}		20.7376	18.3398	24.3655	40.9261	14.5875	12.3115	21.8650
T_0/K	290.00	289.00	368.15	323.15	368.15	248.40	323.15	323.15
T_{min}/K	264.80	258.90	273.15	273.15	273.15	226.80	273.15	273.15
T_{max}/K	290.00	363.60	368.15	368.15	368.15	364.40	368.15	368.15
P_{min}/MPa	10.00	100.00	49.03	49.03	49.03	100.00	49.03	49.03
P_{max}/MPa	130.00	400.00	1176.80	1176.80	1176.80	400.00	1176.80	1176.80
RMSD/kg·m^{-3}	0.320	0.619	0.415	0.718	1.479	0.953	0.777	0.632
$RMSD_r$/%	0.037	0.068	0.046	0.079	0.166	0.107	0.083	0.067
bias/kg·m^{-3}	−0.031	0.001	0.037	0.071	0.117	−0.040	0.067	0.066
N_p	36	23	29	35	30	33	33	34
±	−6	3	−1	−1	2	−3	1	2
s_w	0.830	1.085	1.075	1.075	0.902	1.077	0.975	1.062

	2,7-dimethyl-2-octanol	cyclopentanol	cyclohexanol	1,2-ethanediol	1,2-propanediol	1,3-propanediol	1,2,3-propanetriol	1,3-butanediol
c_0	0.083212	0.086191	0.061342	0.095014	0.098352	0.096354	0.114255	0.115162
b_0/MPa	123.1681	121.4409	100.7280	258.3450	249.4084	231.1928	527.4930	290.6718
b_1/MPa·K^{-1}	−120.2454	−2.8413		−101.5158	−56.5748	−62.9969	−133.6162	−94.8613
b_2/MPa·K^{-2}	57.6528	149.6110		12.7583	−25.9646	−69.2349	4.4891	−7.9105
T_0/K	298.15	324.90	313.20	298.15	273.15	323.15	273.15	273.15
T_{min}/K	298.15	273.30	313.20	298.15	273.15	273.15	223.15	233.15
T_{max}/K	353.15	324.90	313.20	378.15	368.15	368.15	368.15	303.15
P_{min}/MPa	19.61	10.00	10.00	0.69	49.03	20.00	20.00	49.03
P_{max}/MPa	196.13	230.00	30.00	200.00	588.40	1176.80	686.47	274.59
RMSD/kg·m^{-3}	0.448	0.581	0.120	0.344	0.554	0.735	0.796	0.067
$RMSD_r$/%	0.054	0.060	0.013	0.031	0.051	0.063	0.061	0.006
bias/kg·m^{-3}	−0.062	−0.019	−0.014	0.027	0.043	0.052	−0.253	−0.001
N_p	40	68	3	41	24	41	133	56
±	0	4	−1	9	−4	3	−51	−2
s_w	1.098	1.032	0.910	1.003	1.011	0.908	1.063	0.972

Table 3 (Continued)

	1,5-pentanediol	2-methyl-2,4-pentanediol	3-oxa-1-butanol	3-oxa-1-heptanol	3-oxa-1,5-pentanediol	3,6-dioxa-1-octanol	3-methyl-1-hydroxy benzene	4-allyl-2-methoxy-1-hydroxy benzene
c_0	0.134992	0.107761	0.095161	0.091296	0.100758	0.157534	0.075527	0.085560
c_1/K^{-1}							0.007078	
b_0/MPa	360.0408	185.5936	133.7094	118.4045	255.9953	274.4981	126.4379	185.5742
b_1/MPa·K^{-1}	−118.6652	−79.6870	−78.0617	−73.4625	−82.7560	−138.0063	−53.8417	
b_2/MPa·K^{-2}		−6.6494	8.2277	19.5546	36.6852	15.7517	6.2102	
T_0/K	273.15	273.15	298.15	298.15	323.15	298.15	323.15	273.15
T_{min}/K	253.15	223.15	298.15	288.15	273.15	298.15	298.15	273.15
T_{max}/K	308.15	303.15	343.15	348.15	368.15	448.15	503.15	273.15
P_{min}/MPa	49.03	49.03	10.00	2.55	49.03	0.41	0.69	49.03
P_{max}/MPa	274.59	274.59	300.00	380.68	1176.80	25.25	400.00	490.33
RMSD/kg·m^{-3}	0.045	0.115	0.041	0.289	0.749	0.188	0.230	0.142
RMSD$_r$/%	0.004	0.011	0.004	0.031	0.062	0.019	0.023	0.012
bias/kg·m^{-3}	−0.001	−0.005	0.001	0.080	0.019	−0.012	−0.014	−0.016
N_p	45	63	52	138	33	62	225	7
±	−1	−7	0	28	9	−2	15	−1
s_w	1.021	1.028	0.969	0.983	0.979	1.029	1.014	0.980

[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.

check of aconsistency of the fits with independent data. The literature values of isothermal compressibility used for the comparison in Table 6 are the values obtained mostly from speed-of-sound measurements and were either taken directly from the papers or calculated from the equation

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

where M, u, α_P, and c_P are 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 6.

In the following, a brief commentary is given for each class of substances.

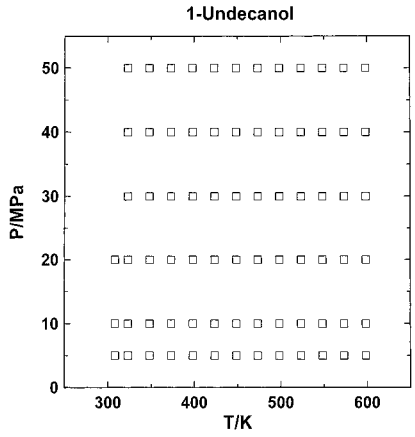
Higher 1-Alkanols (C_{11}, C_{12}, C_{14}, C_{16}). One data set was available for all but one 1-alkanol. The fit of data reported for 1-undecanol by Naziev et al. [90-naz/sha] yields large positive deviations from directly measured isothermal compressibilities [79-dia/tar] (about 13% in an average, Table 6). This indicates that values calculated at high temperatures from the fit for 1-dodecanol might be also unreliable; the values by [90-naz/sha] at the temperature range where $P-\rho-T$ data from other sources ([89-mat/mak], [93-gar/ban]) were available were rejected and the final fit (Table 3) based mainly on the retained values ([89-mat/mak], [93-gar/ban]) in the close-to-ambient temperature range yields good agreement with isothermal compressibilities [79-dia/tar] (average deviation −1.1%, see Table 6). Two fits of densities $\rho(T,P_{ref})$ are presented in Appendix II for 1-dodecanol; the fit of data by 90-naz/sha gives significantly lower values (by 1.0 kg·m^{-3} at T = 298.15 K and 3.9 kg·m^{-3} at T = 498.15 K) than that of data by 76-hal/ell, while the average deviations of reference densities $\rho(T,P_{ref})$ reported by 89-mat/mak and 93-gar/ban from smoothed values [76-hal/ell] are 0.27 kg·m^{-3} and 0.28 kg·m^{-3} (both positive), respectively. Good agreement of $P-\rho-T$ data by 89-mat/mak with literature values of isothermal compressibility indicates that also $P-\rho-T$ data for 1-tetradecanol and 1-hexadecanol from this source might be of good reliability.

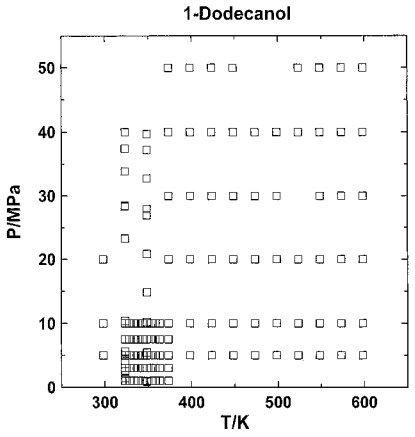
Secondary, Tertiary, and Branched Alkanols. The agreement of isothermal compressibilities calculated from the fit in Table 3 for 2-propanol is quite reasonable at temperatures below 313.15 K, where negative deviations less than 5% from the literature data are observed (Table 6). It should be noted that sound speed values reported by Islam and Quadri [87-isl/qua] are likely to be too low, yielding compressibilities larger than those from other sources. At higher temperatures where the fit is based primarily on $P-\rho-T$ data reported in 80-gol/vas and 87-kub/tan the deviations reach large values (up to −23%). A tentative fit of data reported by 87-kub/tan yielded values of isothermal compressibility lower (by 1.2% on average) than those calculated from the fit in Table 3.

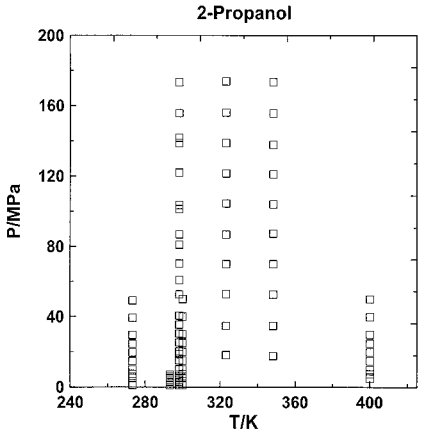
The mutual agreement of the retained data sets for 2-butanol and 2-methyl-1-propanol (isobutanol) is below 0.1%, and also the deviations of calculated isothermal compressibilities from the literature values (Table 6) are satisfactory, being below 5% (2-butanol) and 3% (2-methyl-1-propanol).

Values reported by Wappmann et al. [95-wap/kar] for 2-pentanol and 3-pentanol are consistent with the low-pressure F-type values obtained by Sahli et al. [76-sah/gag] by centrifugation. The authors 95-wap/kar fitted their data using the Tait equation using the lowest experimental pressure 10 MPa as a reference line and found a maximum deviation of 0.5% from the fits. In our fits we have employed the reference densities extrapolated to P = 0.1 MPa from their fits (see also Appendix I). The deviations of those extrapolated values from densities reported in 66-trc are, however, large, being on average 1.3 kg·m^{-3} (2-pentanol, negative) and 1.0 kg·m^{-3} (3-pentanol, positive). When we fit eq 1, it was observed that the compressed-liquid density values for temperatures T = 342.9 K (2-pentanol) and T = 343.1 K (3-pentanol) showed large negative deviations from the fits of values for other isotherms (10 kg·m^{-3} and 2 kg·m^{-3}, respectively). After the values for these two isotherms were rejected (in the case of 2-pentanol for pressures above 60 MPa), the fits representing the data by 95-wap/kar with average deviations below 0.04% were obtained (see Table 4). The comparison of isothermal compressibilities presented in Table 6 is not of a high significance since the F-type values from 76-sah/gag covering the pressure range below that of data from 95-wap/kar were included in the correlated data set.

In the database there was only one data set per substance available for 2-methyl-1-butanol, 2-methyl-2-bu-


1-Undecanol
P/MPa
T/K


1-Dodecanol
P/MPa
T/K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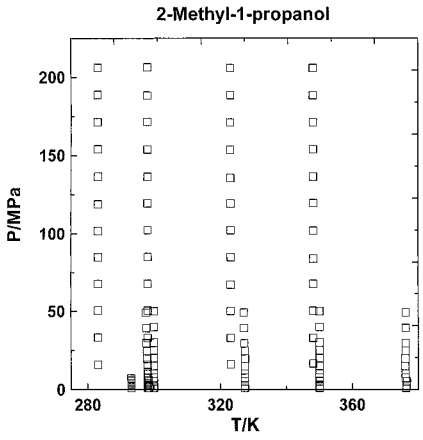
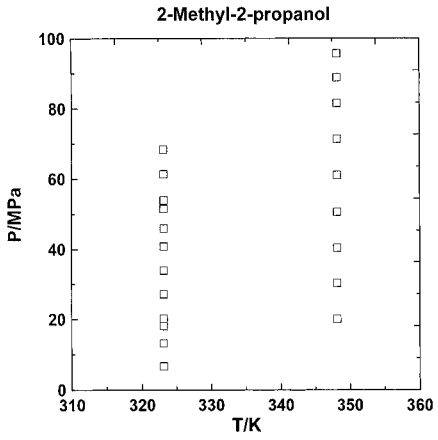
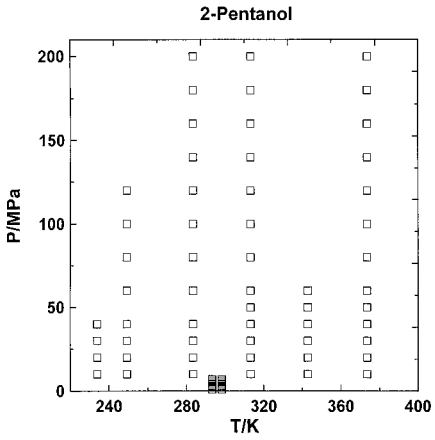
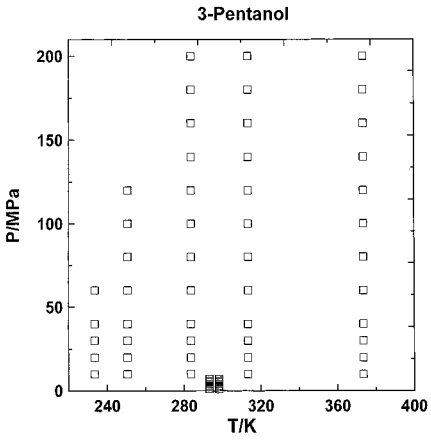
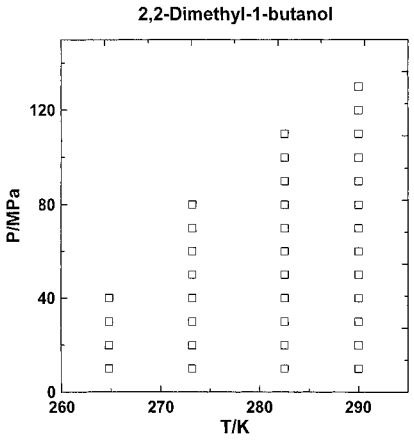
P/MPa
T/K

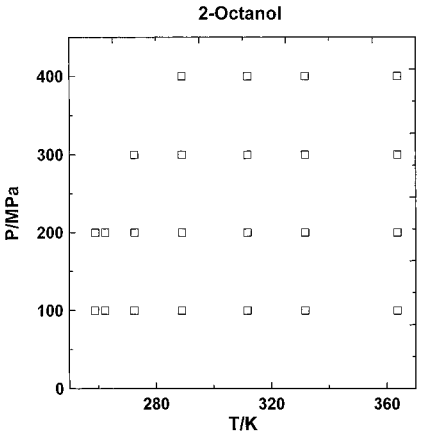

2-Methyl-1-propanol
P/MPa
T/K

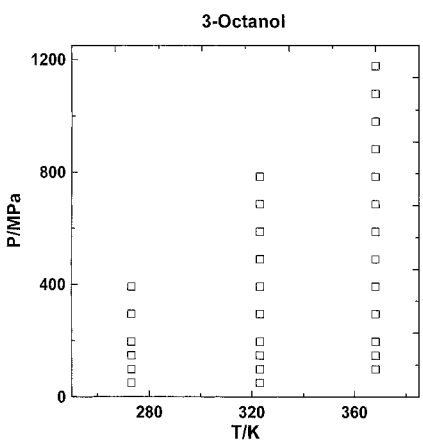

2-Methyl-2-propanol
P/MPa
T/K

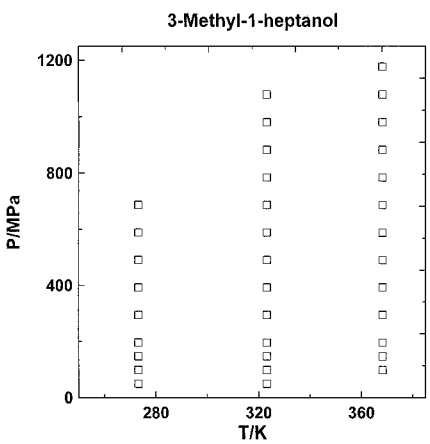

2-Pentanol
P/MPa
T/K

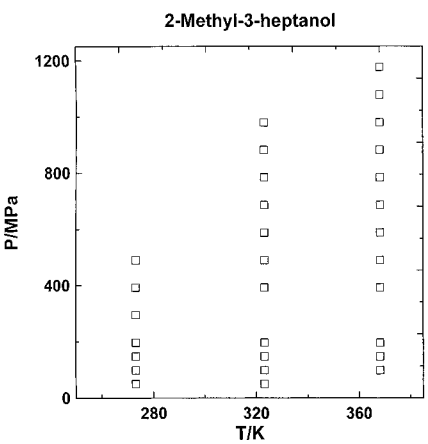

3-Pentanol
P/MPa
T/K


2,2-Dimethyl-1-butanol
P/MPa
T/K


2-Octanol
P/MPa
T/K


3-Octanol
P/MPa
T/K


3-Methyl-1-heptanol
P/MPa
T/K


2-Methyl-3-heptanol
P/MPa
T/K

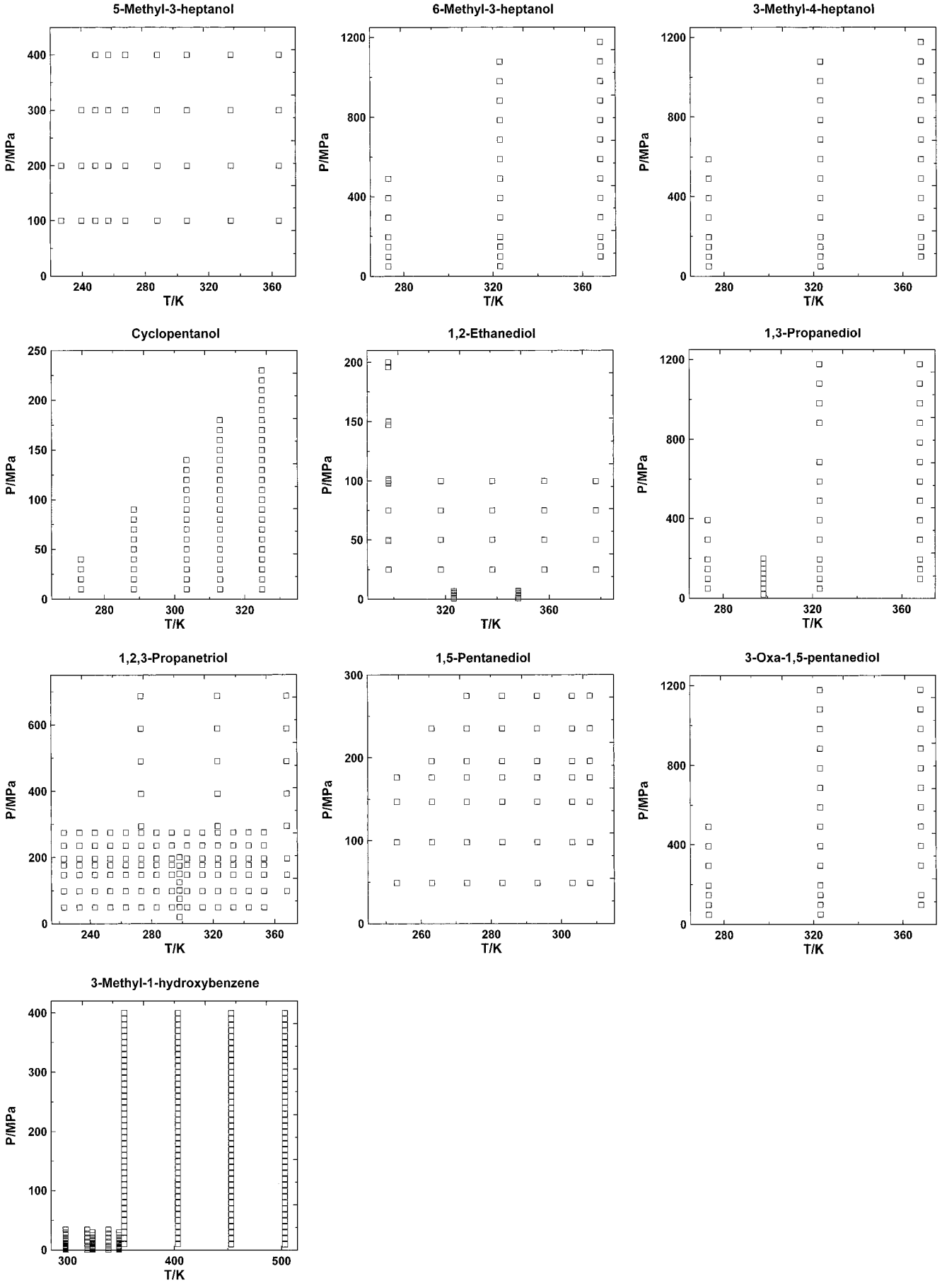


Figure 1. Temperature and pressure coordinates of data points retained in the correlations for the fits in Table 3 where $T-P$ areas of retained data points are not rectangular.

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]
				1-Undecanol						
90-naz/sha	308.15	598.15	5.0	50.0	0.814	0.116	−0.098	75	−11	o
				1-Dodecanol						
89-mat/mak	323.15	348.15	0.9	40.0	0.084	0.010	0.056	21	11	o
90-naz/sha	298.15	598.15	5.0	50.0	1.038	0.146	0.398	60	32	o
93-gar/ban	323.15	373.15	1.0	10.0	0.154	0.019	−0.069	50	−12	o
				1-Tetradecanol						
89-mat/mak	323.15	348.15	0.6	39.7	0.091	0.011	−0.003	22	−2	o
				1-Hexadecanol						
89-mat/mak	348.15	348.15	0.3	40.1	0.077	0.009	−0.002	10	0	o
				2-Propanol (Isopropyl Alcohol)						
31-bri					2.582	0.304	−2.159	8	−8	(o)
42-bri								0	0	e
56-stu					3.506	0.421	−3.137	8	−8	o
56-stu					4.085	0.489	−4.085	1	−1	o
63-gol/bag					7.443	1.066	−4.262	56	−48	e
63-gol/bag					8.134	1.162	−5.151	36	−36	(o)
71-ham/smi					2.735	0.327	−2.735	1	−1	o
71-tse/sti								0	0	e
76-sah/gag	293.15	298.15	1.0	7.0	0.007	0.001	0.000	14	0	o
77-mor/inu	298.15	298.15	10.1	141.9	0.262	0.031	0.060	9	3	o
77-mor/mor	298.15	298.15	101.3	101.3	0.186	0.022	0.186	1	1	o
78-amb/cou					3.280	0.482	2.097	21	13	e
79-gol/vas					3.764	0.529	−0.252	43	21	e
79-zol/gol	273.15	273.15	1.1	49.1	0.539	0.066	0.516	11	11	e
80-gol/vas	300.00	400.00	1.0	50.0	0.607	0.080	0.369	20	12	e
80-rae/fin					4.153	0.504	−1.434	25	−5	e
87-kub/tan	298.15	348.15	17.8	173.9	0.369	0.045	−0.182	30	−10	o
				2-Butanol (*sec*-Butyl Alcohol)						
76-sah/gag	293.15	298.15	1.0	7.0	0.039	0.005	0.037	14	14	o
87-kub/tan	283.15	348.15	15.4	206.5	0.611	0.071	0.477	48	32	o
92-uos/kit	298.15	298.15	50.0	200.0	0.279	0.032	−0.244	4	−4	o
				2-Methyl-1-propanol (Isobutyl Alcohol)						
63-gol/bag					2.521	0.326	2.090	33	29	e
63-gol/bag					2.240	0.284	0.528	30	6	(o)
76-sah/gag	293.15	298.15	1.0	7.0	0.012	0.002	0.002	14	6	o
79-vas/gol	297.66	376.52	1.1	49.1	0.700	0.090	0.663	33	33	e
79-zol/gol								0	0	e
80-gol/vas	300.00	350.00	1.0	50.0	0.769	0.098	0.722	22	22	e
87-kub/tan	283.15	348.15	15.8	206.5	0.265	0.031	−0.051	48	−6	o
				2-Methyl-2-propanol (*tert*-Butyl Alcohol)						
87-kub/tan	323.15	348.15	6.7	95.7	0.121	0.015	0.009	21	−1	o
				2-Pentanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.186	0.023	−0.162	14	−14	o
95-wap/kar	234.00	373.40	10.0	200.0	0.340	0.039	0.031	56	10	e[c]
				3-Pentanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.135	0.016	−0.116	14	−14	o
95-wap/kar	233.60	373.40	10.0	200.0	0.295	0.035	0.089	49	11	e[c]
				2-Methyl-1-butanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.004	0.000	0.001	14	2	o
				3-Methyl-1-butanol (Isoamyl Alcohol)						
76-sah/gag	293.15	298.15	1.0	7.0	0.032	0.004	0.019	14	4	o
81-gol/vas	273.15	386.90	1.1	49.1	0.795	0.102	−0.278	21	−7	e
				2-Methyl-2-butanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.003	0.000	0.000	14	0	o
				3-Methyl-2-butanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.002	0.000	0.000	14	2	o
				2-Methyl-2-pentanol						
76-sah/gag	293.15	298.15	1.0	7.0	0.004	0.001	0.000	14	−2	o
				4-Methyl-2-pentanol						
92-uos/kit	298.15	298.15	50.0	200.0	0.250	0.029	0.004	4	2	o
				2,2-Dimethyl-1-butanol						
91-ede/bar	264.80	290.00	10.0	130.0	0.320	0.037	−0.031	36	−6	o
				2-Octanol						
68-joh/dan	258.90	363.60	100.0	400.0	0.619	0.068	0.001	23	3	o
				3-Octanol						
33-bri	273.15	368.15	49.0	1176.8	0.415	0.046	0.037	29	−1	o
68-joh/dan[b]					6.313	0.688	−5.785	26	−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]
				3-Methyl-1-heptanol						
33-bri	273.15	368.15	49.0	1176.8	0.718	0.079	0.071	35	−1	o
				2-Methyl-3-heptanol						
33-bri	273.15	368.15	49.0	1176.8	1.479	0.166	0.117	30	2	o
68-joh/dan[b]					5.241	0.574	−2.370	37	−11	o
				5-Methyl-3-heptanol						
68-joh/dan	226.80	364.40	100.0	400.0	0.953	0.107	−0.040	33	−3	o
				6-Methyl-3-heptanol						
33-bri	273.15	368.15	49.0	1176.8	0.777	0.083	0.067	33	1	o
				3-Methyl-4-heptanol						
33-bri	273.15	368.15	49.0	1176.8	0.632	0.067	0.066	34	2	o
				2,7-Dimethyl-2-octanol						
55-kus	298.15	353.15	19.6	196.1	0.448	0.054	−0.062	40	0	o
				Cyclopentanol						
82-wis/wue	273.30	324.90	10.0	230.0	0.581	0.060	−0.019	68	4	o
				Cyclohexanol						
90-rie/sch	313.20	313.20	10.0	30.0	0.120	0.013	−0.014	3	−1	o
				1,2-Ethanediol (Ethylene Glycol)						
32-bri					4.537	0.403	1.825	11	3	o[d]
41-gib/loe	298.15	378.15	25.0	100.0	0.104	0.009	0.049	20	4	o
71-ham/smi					3.074	0.270	−3.074	1	−1	o
81-dic								0	0	o
82-kob/nis	298.15	298.15	49.0	196.1	0.479	0.041	0.456	4	4	o
83-nak/miy	298.15	298.15	101.3	101.3	0.049	0.004	−0.049	1	−1	o
90-miy/tak	298.15	298.15	50.0	200.0	0.109	0.009	0.032	4	2	o
90-won/hay	323.20	348.20	0.7	6.9	0.553	0.051	−0.148	12	0	o
				1,2-Propanediol						
32-bbri	273.15	368.15	49.0	588.4	0.544	0.050	0.013	23	−5	o[d]
71-ham/smi	303.15	303.15	101.3	101.3	0.741	0.069	0.741	1	1	o
90-miy/tak[b]					3.333	0.307	3.260	4	4	o
				1,3-Propanediol						
32-bri	273.15	368.15	49.0	1176.8	0.828	0.071	0.063	32	2	o[d]
83-nak/miy	298.15	298.15	101.3	101.3	0.210	0.019	0.210	1	1	o
90-miy/tak[b]	298.15	298.15	20.0	200.0	0.126	0.012	−0.011	8	0	o
				1,2,3-Propanetriol (Glycerine)						
26-bri					3.090	0.234	0.885	3	1	o
32-bri	273.15	368.15	49.0	686.5	1.651	0.126	−0.772	26	−12	o[d]
57-wal/ric								0	0	o
69-mcd/for	223.15	353.15	49.0	274.6	0.362	0.028	−0.145	98	−42	o
81-dic								0	0	o
83-nak/miy	298.15	298.15	101.3	101.3	0.191	0.015	0.191	1	1	o
90-miy/tak[b]	298.15	298.15	20.0	200.0	0.269	0.021	0.058	8	2	o
				1,3-Butanediol						
69-mcd/for	233.15	303.15	49.0	274.6	0.067	0.006	−0.001	56	−2	o
				1,5-Pentanediol						
69-mcd/for	253.15	308.15	49.0	274.6	0.045	0.004	−0.001	45	−1	o
				2-Methyl-2,4-pentanediol (Hexylene Glycol)						
69-mcd/for	223.15	303.15	49.0	274.6	0.115	0.011	−0.005	63	−7	o
				3-Oxa-1-butanol (2-Methoxyethanol)						
87-led	298.15	343.15	10.0	300.0	0.041	0.004	0.001	52	0	o
				3-Oxa-1-heptanol (2-Butoxyethanol)						
93-mal/woo	288.15	348.15	2.6	380.7	0.289	0.031	0.080	138	28	o
				3-Oxa-1,5-pentanediol (Diethylene Glycol)						
32-bri	273.15	368.15	49.0	1176.8	0.749	0.062	0.019	33	9	o[d]
				3,6-Dioxa-1-octanol (Diethylene Glycol Monoethyl Ether)						
77-akh/ima	298.15	448.15	0.4	25.2	0.188	0.019	−0.012	62	−2	o
				3-Methyl-1-hydroxybenzene (*m*-Cresol)						
68-bel/erg					5.028	0.487	4.244	11	11	o
88-sid/tej	298.20	338.20	0.7	34.5	0.228	0.022	−0.136	20	−12	o
95-cha/lee	298.15	348.15	1.0	30.0	0.076	0.007	0.025	45	7	o
95-ran/lew	353.15	503.15	10.0	400.0	0.258	0.026	−0.010	160	20	o
				4-Allyl-2-methoxy-1-hydroxybenzene (Eugenol)						
32-bri	273.15	273.15	49.0	490.3	0.142	0.012	−0.016	7	−1	o

[a] o, (o), from the same source as the compressed liquid density data, available for a part of the temperature range only, respectively; e, from the smoothing equation (see Appendix I). [b] See text. [c] Smoothed reference densities (P_{ref} = 0.1 MPa, see Appendix I) were obtained by fitting the extrapolated values (extrapolation along each experimental isotherm using Tait equation). [d] Relative volumes $V(T,P)/V(T = 273.15$ K, $P = 0.1$ MPa) presented in 32-bri were recalculated to $V(T,P)/V(T, P = 0.1$ MPa), $T > 273.15$ K, using both $\rho(T = 273.15$ K, $P = 0.1$ MPa) given in the paper and $V(T = 368.15$ K, $P = 0.1$ MPa)$/V(T = 273.15$ K, $P = 0.1$ MPa) obtained by extrapolation of values for the isotherm $T = 368.15$ K using the Tait equation.

Table 5. Parameters c_i, b_i, and T_0 of Eq 1 Fitted to Data from 76-sah/gag,[a] in the Temperature and Pressure Ranges T_{min} = 293.15 K, T_{max} = 298.15 K and P_{min} = 1 MPa, P_{max} = 7 MPa, and Absolute Root Mean Square Deviations, RMSD

	2-propanol	2-butanol	2-methyl-1-propanol	2-pentanol	3-pentanol	3-methyl-1-butanol
c_0	0.075918	0.067186	0.065886	0.073077	0.060829	0.070294
b_0/MPa	67.2050	68.5712	52.4401	72.6208	74.8267	86.2540
b_1/MPa·K^{-1}	−40.1048	−45.4687	−48.2637	−39.1933	−58.8411	−43.2323
T_0/K	298.15	298.15	323.15	313.20	283.60	273.15
RMSD/kg·m^{-3}	0.003	0.004	0.003	0.003	0.003	0.003

[a] For 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-2-butanol, and 2-methyl-2-pentanol, see Table 3.

tanol, 3-methyl-2-butanol, and 2-methyl-2-pentanol [76-sah/gag]. Results of the fits of data for other alkanols presented in [76-sah/gag] (2-propanol, 2-butanol, 2-methyl-1-propanol, 2-pentanol, 3-pentanol, and 3-methyl-1-butanol) are given separately in Table 5. The fits (Tables 3 and 5) are based on the F-type values of the specific volume calculated from smoothing equations presented by Sahli et al. [76-sah/gag], and therefore the deviations (RMSD, $RMSD_r$) are low and do not reflect the accuracy of the experimental data. Isothermal compressibilities, β_T(T = 293.15 or 298.15 K, P = 0.1 MPa) calculated from the fits of data from 76-sah/gag by eq 1 for all those alkanols are, however, slightly lower than smoothed values reported by Sahli et al. [76-sah/gag]; deviations vary from −2.4% (2-methyl-1-butanol) to −0.5% (2-butanol), and an average deviation is −1.4% for all alkanols. It should be noted that the parameters reported in Table 2 of the reference 76-sah/gag for the polynomial function $\beta_T = f(P)$ (eq 1 in the reference) correspond probably to pressure in MPa, not in Pa as would follow from dimensions of the parameters in the table.

Isothermal compressibilities of 3-methyl-1-butanol calculated from the fit in Table 3 agree reasonably (deviations below 5%) with the literature data for temperatures below 308.15 K. At higher temperatures the agreement is likely to be worse. It should be pointed out that the isothermal compressibilities based on sound speeds from 87-isl/qua are higher (see also the discussion for 2-propanol above) than data from other sources (see rows for T = 303.15 K and T = 308.15 K in Table 6) by about 10%.

Johari and Dannhauser [68-joh/dan] presented compressed-liquid density data for several isomeric octanols (see Table 2) in the form of the equation $(\rho_T)_P = (\rho_0)_P - A_P(T - 273.15)$ and reported the values of parameters $(\rho_0)_P$ and A_P for four pressures (0.1, 100, 200, 300, and 400 MPa) stating that their experimental values determined with the accuracy of 1 kg·m^{-3} are represented within ±1% by the equation. The fits of the F-type values generated from their equation show, naturally, much lower deviations (2-octanol, 5-methyl-3-heptanol, see Tables 3 and 4) which should not be misinterpreted; the uncertainty of the values calculated from the fits cannot be lower than the value declared by the authors (1%). On the other hand, isothermal compressibilities calculated from the fit for 2-octanol are in surprisingly good agreement with the literature data in the close-to-ambient temperature range (1.5% in an average, see Table 6). The agreement of $P-\rho-T$ data by 68-joh/dan with Bridgman's values for 3-octanol and 2-methyl-3-heptanol [33-bri] is still within the limit of 1% (Table 4); the data by 68-joh/dan were, however, rejected, preferring the directly measured values by Bridgman [33-bri]. The fits of F-type values by 68-joh/dan for those two alkanols resulted in the following data.

3-Octanol: c_0 = 0.088 122; b_0 = 76.2431 MPa; b_1 = −40.0065 MPa·K^{-1}; b_2 = 20.5866 MPa·K^{-2}; T_0 = 368.15 K; T_{min} = 250.90 K; T_{max} = 361.10 K; P_{max} = 400.00 MPa; RMSD = 1.035 kg·m^{-3}; $RMSD_r$ = 0.114%; bias = 0.006 kg·m^{-3}; N_p = 26; ± = 2.

2-Methyl-3-heptanol: c_0 = 0.090 369; b_0 = 81.4339 MPa; b_1 = −40.3321 MPa·K^{-1}; b_2 = 10.2694 MPa·K^{-2}; T_0 = 368.15 K; T_{min} = 216.40 K; T_{max} = 363.50 K; P_{max} = 400.00 MPa; RMSD = 1.470 kg·m^{-3}; $RMSD_r$ = 0.159%; bias = 0.063 kg·m^{-3}; N_p = 37; ± = 9.

Cycloalkanols. One data set per substance was available for cyclopentanol and cyclohexanol. The isothermal compressibility calculated from the fit for cyclopentanol agrees well with the literature value (deviation 3.2%, Table 6). The agreement for cyclohexanol is similar; however, the deviation from the value evaluated from calorimetric measurements by Petit and Ter Minassian [74-pet/ter] is rather large (−9.9%).

Diols and Triols. Values retained in the fit for 1,2-ethanediol (five data sets) are in mutual agreement within 0.05% (on average, see Table 4). F-type data from 41-gib/loe were generated using the parameters of both the Tait equation reported by the authors separately for each experimental temperature and the parameters of the third-order polynomial in temperature given in the same source for specific volume at atmospheric pressure. Isothermal compressibilities calculated from the fit agree well with literature values (deviations within ±2%, Table 6).

The deviations in isothermal compressibility are much larger in the case of 1,2-propanediol (−14% in an average, Table 6) where the values from the sources 32-bri and 71-ham/smi were retained in the final fit. The maximum pressure of the retained data set reported by Bridgman [32-bri] was decreased since large deviations were observed at high pressures. It should be noted that the data from 32-bri and 71-ham/smi were rejected for 1,2-ethanediol, while the values by Miyamoto et al. [90-miy/tak] are in very good agreement with isothermal compressibilities taken from the literature for this substance. Therefore, an additional fit was performed for 1,2-propanediol, retaining only the data set [90-miy/tak] which resulted in c_0 = 0.085 532, b_0 = 179.0139 MPa, T_{min} = T_{max} = 298.15 K, P_{max} = 200.00 MPa, RMSD = 0.072 kg·m^{-3}, $RMSD_r$ = 0.007%, bias = 0.000 kg·m^{-3}, N_p = 4, ± = 0. The isothermal compressibility calculated from the fit, β_T(T = 298.15 K, P = 0.1 MPa) = 0.478 GPa^{-1}, agrees excellently with the value reported by 86-kar/rod (Table 6), differing only by −0.8%.

The agreement in isothermal compressibilities for 1,3-propanediol is good (below 2%, see Table 6) in the temperature range close to 298.15 K, where the fit is based on isothermal (T = 298.15 K) $P-\rho-T$ data reported in 83-nak/miy and 90-miy/tak. Larger deviations (up to ±6%) are observed at other temperatures where the fit is based on the directly measured data from 32-bri. The function $B(T)$ (eq 3) is, contrary to the usual convex shape, concave, showing the maximum at T = 278 K, which indicates a mutual inconsistency of the retained data sets. Similarly as in the case of 1,2-propanediol, an additional fit of data from 90-miy/tak was performed: c_0 = 0.092 853; b_0 = 231.8143 MPa; T_{min} = T_{max} = 298.15 K; P_{max} = 200.00 MPa; RMSD = 0.080 kg·m^{-3}; $RMSD_r$ = 0.007%; bias = 0.001 kg·m^{-3}; N_p = 8; ± = 2. The isothermal compressibility calculated from the fit, β_T(T = 298.15 K, P = 0.1 MPa) =

Table 6. 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 (Eq 1) with Literature Data

	β_T/GPa^{-1}			
T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref
		1-Undecanol		
308.15	0.84 ± 0.03	0.776	16.7	79-dia/tar[c]
318.15	0.89 ± 0.03	0.803	11.2	79-dia/tar[c]
333.15	0.97 ± 0.03	0.880	10.7	79-dia/tar[c]
		1-Dodecanol		
298.15	0.702 ± 0.004	0.709	−1.0	79-dia/tar[c]
308.15	0.741 ± 0.004	0.747	−0.8	79-dia/tar[c]
318.15	0.783 ± 0.005	0.794	−1.4	79-dia/tar[c]
333.15	0.853 ± 0.005	0.864	−1.3	79-dia/tar[c]
		2-Propanol		
298.15	1.123 ± 0.007	1.148	−2.2	93-ami/ara,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.167	−3.8	86-mou/nai,[d] 76-hal/ell,[e] 96-zab/ruz[f]
303.15	1.159 ± 0.008	1.197	−3.2	93-ami/ara,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.190	−2.6	93-sri/nai,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.313	−11.7	87-isl/qua,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.186	−2.3	66-kat/shi[c]
308.15	1.197 ± 0.008	1.261	−5.0	93-ami/ara,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.251	−4.3	82-kar/red,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.364	−12.2	87-isl/qua,[d] 76-hal/ell,[e] 96-zab/ruz[f]
313.15	1.239 ± 0.009	1.427	−13.2	87-isl/qua,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		1.332	−7.0	66-kat/shi[c]
318.15	1.28 ± 0.01	1.491	−14.1	87-isl/qua,[d] 76-hal/ell,[e] 96-zab/ruz[f]
323.15	1.33 ± 0.01	1.505	−11.6	66-kat/shi[c]
333.15	1.45 ± 0.02	1.729	−16.1	66-kat/shi[c]
343.15	1.58 ± 0.02	2.039	−22.5	66-kat/shi[c]
		2-Butanol		
293.15	0.928 ± 0.006	0.966	−3.9	76-sah/gag[c]
298.15	0.957 ± 0.006	0.983	−2.6	76-sah/gag[c]
		1.002	−4.5	88-oka/oga,[d] 76-hal/ell,[e] 96-zab/ruz[f]
		2-Methyl-1-propanol		
293.15	0.977 ± 0.006	0.993	−1.6	76-sah/gag[c]
298.15	1.008 ± 0.006	1.034	−2.5	76-sah/gag[c]
		1.033	−2.5	88-oka/oga,[d] 66-trc,[e] 96-zab/ruz[f]
		1.029	−2.0	93-ami/ara,[d] 66-trc,[e] 96-zab/ruz[f]
303.15	1.040 ± 0.006	1.068	−2.6	82-ven/dha,[d] 66-trc,[e] 96-zab/ruz[f]
		1.068	−2.6	93-sri/nai,[d] 66-trc,[e] 96-zab/ruz[f]
		1.068	−2.6	93-ami/ara,[d] 66-trc,[e] 96-zab/ruz[f]
308.15	1.075 ± 0.007	1.107	−2.9	93-ami/ara,[d] 66-trc,[e] 96-zab/ruz[f]
		1.107	−2.9	82-kar/red,[d] 66-trc,[e] 96-zab/rus[f]
		2-Pentanol		
293.15	0.949 ± 0.005	0.919	3.3	76-sah/gag[c]
298.15	0.980 ± 0.005	0.947	3.5	76-sah/gag[c]
		3-Pentanol		
293.15	0.908 ± 0.006	0.891	1.9	76-sah/gag[c]
298.15	0.940 ± 0.006	0.928	1.3	76-sah/gagc[c]
		3-Methyl-1-butanol		
293.15	0.91 ± 0.01	0.917	−0.8	76-sah/gag[c]
298.15	0.92 ± 0.01	0.942	−2.3	76-sah/gag[c]
		0.939	−2.0	86-mou/nai,[d] 66-trc,[e] 96-zab/ruz[f]
303.15	0.93 ± 0.01	0.940	−1.1	82-ven/dha,[d] 66-trc,[e] 96-zab/ruz[f]
		0.946	−1.7	93-sri/nai,[d] 66-trc,[e] 96-zab/ruz[f]
		1.072	−13.2	87-isl/qua,[d] 66-trc,[e] 96-zab/ruz[f]
308.15	0.95 ± 0.02	0.978	−2.9	82-kar/red,[d] 66-trc,[e] 96-zab/ruz[f]
		1.120	−15.2	87-isl/qua,[d] 66-trc,[e] 96-zab/ruz[f]
313.15	0.96 ± 0.02	1.176	−18.4	87-isl/qua,[d] 66-trc,[e] 96-zab/ruz[f]
318.15	0.98 ± 0.02	1.228	−20.2	87-isl/qua,[d] 66-trc,[e] 96-zab/ruz[f]
		2-Methyl-2-butanol		
293.15	1.011 ± 0.002	1.004	0.7	71-des/bha,[d] 66-trc,[e] 96-zab/ruz[f]
		2-Octanol		
298.15	0.835 ± 0.014	0.810	3.1	82-aww/pet,[d] 68-trc,[e] 96-zab/ruz[f]
		0.826	1.1	93-ami/ara,[d] 68-trc,[e] 96-zab/ruz[f]
303.15	0.861 ± 0.014	0.852	1.1	93-ami/ara,[d] 68-trc,[e] 96-zab/ruz[f]
308.15	0.889 ± 0.015	0.884	0.6	93-ami/ara,[d] 68-trc,[e] 96-zab/ruz[f]
		Cyclopentanol		
298.15	0.648 ± 0.008	0.628	3.2	74-kiy/gro,[d] 88-wis/wue,[e] 96-zab/ruz[f]
		Cyclohexanol		
313.20	0.61 ± 0.03	0.677	−9.9	74-pet/ter[c,g]
		0.638	−4.4	*h*, 80-raj/sub,[e] 96-zab/ruz[f]
		0.644	−5.3	*h*, 84-sip/wie,[e] 96-zab/ruz[f]

Table 6 (Continued)

	β_T/GPa^{-1}			
T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref
		1,2-Ethanediol		
298.15	0.368 ± 0.002	0.360	2.2	86-kar/rod[c]
		0.375	−1.9	91-dou/pal,[d] *i*, 96-zab/ruz[f]
303.15	0.375 ± 0.002	0.380	−1.3	63-art,[d] *i*, 96-zab/ruz[f]
313.15	0.390 ± 0.002	0.387	0.8	86-kar/rod[c]
		0.398	−2.0	63-art,[d] *i*, 96-zab/ruz[f]
323.15	0.406 ± 0.002	0.411	−1.2	63-art,[d] *i*, 96-zab/ruz[f]
333.15	0.423 ± 0.002	0.423	0.0	86-kar/rod[c]
		0.427	−0.9	63-art,[d] *i*, 96-zab/ruz[f]
343.15	0.441 ± 0.002	0.449	−1.8	63-art,[d] *i*, 96-zab/ruz[f]
353.15	0.460 ± 0.002	0.467	−1.5	63-art,[d] *i*, 96-zab/ruz[f]
		1,2-Propanediol		
283.15	0.404 ± 0.004	0.450	−10.2	86-kar/rod[c]
293.15	0.415 ± 0.004	0.469	−11.5	86-kar/rod[c]
298.15	0.421 ± 0.004	0.482	−12.7	86-kar/rod[c]
313.15	0.442 ± 0.005	0.519	−14.8	86-kar/rod[c]
333.15	0.477 ± 0.006	0.567	−21.2	86-kar/rod[c]
		1,3-Propanediol		
278.15	0.392 ± 0.004	0.377	4.0	86-kar/rod[c]
283.15	0.393 ± 0.003	0.382	2.9	86-kar/rod[c]
293.15	0.395 ± 0.001	0.393	0.5	86-kar/rod[c]
298.15	0.397 ± 0.001	0.404	−1.7	86-kar/rod[c]
313.15	0.407 ± 0.004	0.422	−3.6	86-kar/rod[c]
333.15	0.430 ± 0.005	0.456	−5.7	86-kar/rod[c]
		1,2,3-Propanetriol		
293.15	0.222 ± 0.001	0.242	−5.8	29-fre/hub,[d] 69-mcd/for,[e] 96-zab/ruz[f]
		0.238	−4.2	29-fre/hub,[d] 93-cda,[e] 96-zab/ruz[f]
303.15	0.234 ± 0.001	0.248	−5.6	29-fre/hub,[d] 69-mcd/for,[e] 96-zab/ruz[f]
		0.244	−4.1	29-fre/hub,[d] 93-cda,[e] 96-zab/ruz[f]
313.15	0.241 ± 0.001	0.254	−5.1	29-fre/hub,[d] 69-mcd/for,[e] 96-zab/ruz[f]
323.15	0.247 ± 0.001	0.260	−5.0	29-fre/hub,[d] 69-mcd/for,[e] 96-zab/ruz[f]
333.15	0.254 ± 0.001	0.272	−6.6	63-art,[d] 69-mcd/for,[e] 96-zab/ruz[f]
343.15	0.262 ± 0.002	0.280	−6.4	63-art,[d] 69-mcd/for,[e] 96-zab/ruz[f]
353.15	0.270 ± 0.002	0.288	−6.3	63-art,[d] 69-mcd/for,[e] 96-zab/ruz[f]
		3-Oxa-1-butanol		
298.15	0.711 ± 0.001	0.717	−0.8	90-dou/pal,[d] 87-led,[e] 96-zab/ruz[f]
303.15	0.732 ± 0.001	0.731	0.1	95-kri/ram,[d] 87-led,[e] 96-zab/ruz[f]
		3-Oxa-1-heptanol		
298.15	0.770 ± 0.002	0.783	−1.7	90-dou/pal,[d] *j*, 96-zab/ruz[f]
		3-Methyl-1-hydroxybenzene		
323.15	0.597 ± 0.002	0.595	0.3	68-bel/erg,[d] *k*, 96-zab/ruz[f]
363.15	0.739 ± 0.002	0.740	−0.1	68-bel/erg,[d] *k*, 96-zab/ruz[f]

[a] Uncertainty is estimated as ±2*s*, where *s* is a standard deviation derived from a covariance matrix of each fit. [b] $[\beta_T(\text{eq 1}) - \beta_T(\text{lit.})]100/\beta_T(\text{lit.})$. [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] Interpolated value. [h] Sound speed at $T = 313.20$ K was obtained by polynomial interpolation using data from 80-raj/sub. [i] Densities and α_P from 41-gib/loe and 90-won/hay; see Appendix II. [j] Densities and α_P from smoothing equation presented in 93-mal/woo. [k] Densities and α_P from 68-bel/erg, 95-cha/lee, and 95-ran/lew; see Appendix II.

0.400 GPa^{-1}, agrees better (deviation −1.0%) with the literature value reported by 86-kar/rod (Table 6) than that calculated from the fit in Table 3.

Similarly as for 1,2-propanediol, the values reported by Bridgman 32-bri for 1,2,3-propanetriol at pressures higher than 800 MPa were rejected due to large deviations (above 3 kg·m^{-3}). Isothermal compressibilities calculated from the fit in Table 3 are lower by about 6% than selected literature values (Table 6); the compressibility of 1,2,3-propanetriol is, however, low compared to other substances and thus small absolute deviations result in rather large relative ones. At temperatures around 298.15 K the fit is based on data taken from 83-nak/miy and [90-miy/tak]; the situation is similar to that for 1,2-propanediol and 1,3-propanediol. Therefore, we present the results of the additional fit of data for 1,2,3-propanetriol from 90-miy/tak: $c_0 = 0.098\,021$; $b_0 = 413.7963$ MPa; $T_{min} = T_{max} = 298.15$ K; $P_{max} = 200.00$ MPa; RMSD = 0.196 kg·m^{-3}; $RMSD_r = 0.015\%$; bias = −0.033 kg·m^{-3}; $N_p = 8$; ± = 0. The isothermal compressibility calculated from this fit, β_T(T = 298.15 K, P = 0.1 MPa) = 0.237 GPa^{-1}, differs from that given by the fit in Table 3 (β_T(T = 298.15 K, P = 0.1 MPa) = 0.231 GPa^{-1}) by 2.6% and is in better agreement (deviation −3.3%) with the value 0.245 GPa^{-1} obtained by a polynomial interpolation using literature values for 293.15, 303.15, and 313.15 K from Table 6 ([29-fre/hub], [69-mcd/for], [96-zab/ruz]).

Only one value was found for 1,4-butanediol ([71-ham/smi]; $\{\rho(P = 101.3\text{ MPa})/\rho(P = 0.1\text{ MPa}) - 1\} = 0.0332$ at $T = 303.15$ K), and therefore no correlation was performed.

McDuffie et al. [69-mcd/for] presented the parameters of the Tait equation along with the parameters of the straight-line function representing densities at atmospheric pressure (see Appendix II) for four polyols: 1,2,3-propanetriol, 1,3-butanediol, 1,5-pentanediol, and 2-methyl-2,4-pentanediol, stating that the uncertainty of the values calculated from their fits is about 1 part in 2000 (0.05%). The relative density values calculated from their fit for 1,2,3-propanetriol agree with other retained data within this limit (Table 4). The fits performed for the three diols

Table A-1. Parameters, a_i, of Functions A-1 and A-2 Used for the Fits in Table 3, Critical Densities, ρ_c, Critical Temperatures, 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

	2-propanol	2-methyl-1-propanol	2-pentanol	3-pentanol	3-methyl-1-butanol
eq	A-1	A-1	A-1	A-2	A-2
a_0	0.624542	−1.230509	−1.270940	1015.0351	1202.4465
a_1	6.189375	13.569579	12.973096	−61.61612	−286.2512
a_2	−6.790392	−16.72639	−15.19684	3.546426	80.933918
a_3	2.490094	7.048178	6.270106	−1.734774	−9.862609
ρ_c/kg·m^{-3} [a]	273.163	271.512	267.932		
T_c/K	508.30	547.78	560.40		
T_{min}/K	243.15	253.15	234.00	233.60	273.15
T_{max}/K	430.00	423.15	433.00	433.10	403.15
RMSD/kg·m^{-3}	0.764	0.129	0.238	0.825	0.188
$RMSD_r$/%	0.093	0.019	0.030	0.107	0.026
bias/kg·m^{-3}	0.172	−0.002	0.000	0.001	−0.022
N_p	15	19	8	8	15
±	−3	1	0	2	1
ref(ρ)	76-hal/ell[b]	66-trc	95-wap/kar[c]	95-wap/kar[c]	66-trc
ref(P_{ref})	83-mcg				

[a] Given with three decimal places since critical densities were calculated from rounded values of critical molar volumes recorded in the database [93-cda]. [b] At T < 298.15 K the data from 66-trc were used. [c] Equations A-1 and A-2 were fitted to values obtained by the extrapolation from elevated pressures to P_{ref} = 0.1 MPa along each experimental isotherm using the Tait equation.

are recorrelations of the F-type data, resulting in a lower $RMSD_r$ which should not be misinterpreted; the expected uncertainty of the relative density calculated from the fits should be the same as that declared by the authors.

Ether Alkanols. Only one data set per substance was found for each of four ether alkanols. The deviations between the values of isothermal compressibility calculated from the fits in Table 3 and the independent data found for two 2-alkoxyethanols are below 1% (3-oxa-1-butanol) and 2% (3-oxa-1-heptanol). No data to evaluate isothermal compressibilities for a comparison were found in the literature for other ether alkanols (3-oxa-1,5-pentanediol, 3,6-dioxa-1-octanol).

Aromatic Hydroxy Derivatives. Two $P-\rho-T$ data sets ([88-sid/tej], [95-cha/lee]) recently measured for 3-methyl-1-hydroxybenzene (*m*-cresol) are, in terms of relative density, in very good mutual agreement (within 0.03% in an average). After the values evaluated from calorimetric measurements [95-ran/lew] at higher temperatures have been retained, the Tait parameter C was allowed to vary with temperature to obtain a good fit. The agreement of isothermal compressibilities calculated from the final fit for two temperatures with available literature data is excellent (deviations below 0.3%). Two errors were found in original data for 3-methyl-1-hydroxybenzene: (i) the value reported in 88-sid/tej for T = 298.2 K and P = 13.79 MPa was rejected due to an obvious typographical error in the original source; (ii) the misprinted temperature value in the fourth column of Table III in 95-ran/lew (435.15 K) was replaced by the correct value 453.15 K before correlations were performed. Compressed-liquid density values by Belinskii and Ergopulo [68-bel/erg] were rejected due to positive deviations higher than 1 kg·m^{-3}. On the other hand, their values at atmospheric pressure agree within 0.22 kg·m^{-3} with data from 95-cha/lee and 95-ran/lew, while the values at atmospheric pressure reported in 88-sid/tej are significantly lower, particularly at lower temperatures (the deviations from the fit presented in Appendix II are −9.5 kg·m^{-3} at 298.2 K, −7.3 kg·m^{-3} at 318.2 K, and 0.3 kg·m^{-3} at 338.2 K).

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Appendix I

Equations Used for $\rho(T,P_{ref}(T)) = \rho(T)$ in Fits by Eq 1 and References to Saturated Vapor Pressure Data. In those cases where the reference density values $\rho(T,P_{ref}(T))$ (see eq 1) were not available in original papers, the two following functions were used for the data sets, denoted by letter "e" or "(o)" in the last column of Table 4 to calculate reference density values

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

$$\rho(T/\mathrm{K})/\mathrm{kg\cdot m^{-3}} = a_0 + a_1(T/100) + a_2(T/100)^2 + a_3(T/100)^3 \quad \text{(A-2)}$$

The values of adjustable parameters a_i obtained by fitting to available data using a weighted least squares method are recorded in Table A-1 along with some characteristics of the fits. Equation A-1 was preferably used in those cases where respective critical parameters (ρ_c, T_c) were available. The reference to the saturated vapor pressure data, $P_{ref}(T)$, used in eq 1 for 2-propanol is also given in Table A-1. The other three substances (1-undecanol, 1-dodecanol, 3-methyl-1-hydroxybenzene) for which the upper temperature limits (T_{max}) of the fits in Table 3 are above normal boiling temperatures are not listed in Table A-1, since original values of density at saturation were available in the original papers ([90-naz/sha], [95-ran/lew]); the vapor pressures were calculated from the smoothing equations given by Ambrose and Walton [89-amb/wal] and McGarry [83-mcg] for 1-alkanols and 3-methyl-1-hydroxybenzene, respectively.

The values of reference density, $\rho(T,P_{ref})$, P_{ref} = 0.101 325 MPa in most cases, reported for the same samples in original literature sources of compressed-liquid density data were exclusively employed for the fits in Table 3 for the substances which are not listed in Table A-1.

Appendix II

Parameters of Smoothing Functions for Original Reference Density Data. Table A-2 summarizes values

Table A-2. Parameters a_i of Smoothing Functions A-1 or A-2 Fitted to Original Reference Density Values ($\rho(T,P_{ref})$), Critical Densities,[a] ρ_c, Critical Temperatures,[a] T_c, Temperature Ranges of Validity, T_{min} and T_{max}, and RMSD of the Fits

eq	a_0	a_1	a_2	a_3	ρ_c/kg·m^{-3}	T_c/K	T_{min}/K	T_{max}/K	RMSD/kg·m^{-3}	ref
					1-Undecanol					
A-1	1.45788	1.39643			260.682	705.00	308.15	598.15	0.538	90-naz/sha
					1-Dodecanol					
A-1	0.79074	2.81286	−0.74347		259.524	717.00	298.15	598.15	0.226	90-naz/sha
A-1	1.07321	2.18775	−0.39164		259.524	717.00	298.15	490.00	0.178	76-hal/ell[b]
					1-Tetradecanol					
A-2	978.893	−32.889	−5.471				313.15	348.15	0.050	89-mat/mak
					1-Hexadecanol					
A-1	0.88623	2.03793			259.023	770.00	328.15	348.15	0.052	89-mat/mak
					2-Butanol					
A-1	2.71801	−4.21219	9.33752	−5.47651	275.549	536.05	293.15	490.00	0.184	76-hal/ell[c]
					2-Methyl-2-propanol					
A-1	2.20574	−1.15221	3.88729	−2.30660	269.537	506.21	300.65	465.00	0.041	83-hal/gun[d]
					2-Methyl-1-butanol					
A-2	1053.59	−80.0					293.15	298.15		76-sah/gag[e]
					2-Methyl-2-butanol					
A-2	1079.95	−92.4					293.15	298.15		76-sah/gag[e]
					3-Methyl-2-butanol					
A-2	1067.18	−85.0					293.15	298.15		76-sah/gag[e]
					2-Methyl-2-pentanol					
A-2	1029.24	−73.6					293.15	298.15		76-sah/gag[e]
					2,2-Dimethyl-1-butanol					
A-2	1115.159	−125.229	9.5158				264.80	290.00	0.139	91-ede/bar
					2-Octanol					
A-2	1044.5	−76.6					258.90	363.60		68-joh/dan[f]
					3-Octanol					
A-2	1061.4	−82.0					250.90	361.10		68-joh/dan[f]
					2-Methyl-3-heptanol					
A-2	1060.1	−80.4					216.40	363.50		68-joh/dan[f]
					5-Methyl-3-heptanol					
A-2	1061.2	−83.0					226.80	364.40		68-joh/dan[f]
					2,7-Dimethyl-2-octanol					
A-2	1053.501	−74.945	−1.011				293.15	358.15	0.036	55-kus
					Cyclopentanol					
A-1	1.73617	0.83515			321.395	619.50	273.30	324.90	0.276	82-wis/wue
					Cyclohexanol					
A-2	933.710						313.20	313.20		90-rie/sch
					1,2-Ethanediol					
A-1	1.77482	1.11208			333.701	790.00	298.15	378.15	0.236	*g*
					1,2,3-Propanetriol					
A-2	1451.2	−65.5					223.15	353.15		69-mcd/for[f,h]
					1,3-Butanediol					
A-2	1198.5	−66.6					223.15	313.15		69-mcd/for[f]
					1,5-Pentanediol					
A-2	1167.1	−60.8					243.15	313.15		69-mcd/for[f]
					2-Methyl-2,4-pentanediol					
A-2	1141.0	−74.9					223.15	313.15		69-mcd/for[f]
					3-Oxa-1-butanol					
A-1	4.39906	−5.34855	3.95913		313.149	577.00	298.15	343.15	0.018	87-led
					3,6-Dioxa-1-octanol					
A-2	1386.757	−191.933	34.177	−3.781			298.15	448.15	0.160	77-akh/ima
					3-Methyl-1-hydroxybenzene					
A-1	2.15404	−0.75174	1.15969		349.969	705.80	288.15	503.15	0.227	*i*

[a] Taken from 93-cda. [b] Average deviations of values by 90-naz/sha, 89-mat/mak, and 93-gar/ban from the fit are 3.58 kg·m^{-3} (negative), 0.27 kg·m^{-3} (positive), and 0.28 kg·m^{-3} (positive), respectively. [c] Values from 87-kub/tan are lower below 323.15 K and higher at 348.15 K (average deviation 0.99 kg·m^{-3}); average deviation of data by 76-sah/gag from the fit is 0.19 kg·m^{-3}. [d] Deviations of values by 87-kub/tan from the fit are −0.10 kg·m^{-3} (323.15 K) and 1.24 kg·m^{-3} (348.15 K). [e] Interpolation between values at 293.15 and 298.15 K. [f] F-type data are presented as the linear function of temperature, $\rho = \rho_0 - A(T - 273.15)$, in the original source. [g] [41-gib/loe], [90-won/hay]. [h] All other $P-\rho-T$ data given as relative quantities. [i] [68-bel/erg], [95-cha/sta], [95-ran/lew]; deviations of values by 88-sid/tej from the fit are −9.5 kg·m^{-3} (298.2 K), −7.3 kg·m^{-3} (318.2 K), and 0.3 kg·m^{-3} (338.2 K).

of adjustable parameters a_i of functions A-1 and A-2 (see Appendix I) 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 (Tables 2 and 3). The functions were not, unlike the equations summarized in

Table A-1, employed in smoothing the compressed-liquid density data and are presented as auxiliary information here, which may be useful particularly for less common substances. The functions enable us to calculate smoothed reference density values to be used in the evaluation of compressed-liquid densities from eq 1.

The fits in Table A-2 are not the fits of critically selected experimental data. Only in several cases are the parameters a_i obtained using either recommended density values taken from the TRC Thermodynamic Tables or data from other reliable sources presented.

Original reference density values for substances not listed in Tables A-1 and A-2 were not reported in the original sources; i.e., relative quantities such as relative density, $\rho(T,P)/\rho(T,P_{ref})$, volume ratio, $V(T,P)/V(T,P_{ref})$, or compression, $\{\rho(T,P)/\rho(T,P_{ref}) - 1\}$, only were presented by researchers.

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