Reviews

$P-\rho-T$ Data of Liquids: Summarization and Evaluation. 3. Ethers, Ketones, Aldehydes, Carboxylic Acids, and Esters

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The published experimental $P-\rho-$T data for 21 ethers, 10 ketones, 9 aldehydes, 9 carboxylic acids, and 25 esters (74 substances) in the liquid phase are summarized and reviewed, and the parameters of the Tait equation are given for 73 substances considered. 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.

Introduction

This work is a continuation of a compilation and critical evaluation of published $P-\rho-T$ data of organic substances in a liquid state. The data for two groups of substances, 1-alkanols (part 1) and *n*-alkanes (part 2), have been already reviewed and evaluated ([94-cib/zik], [96-cib/hne]). With these classes of substances, the density data at atmospheric pressure, $\rho(T,P_{ref} = 0.1$ MPa), or at saturation, $\rho(T,P_{ref} = P_{sat})$, had been critically evaluated [93-cib]. In this work the published experimental values of relative density, $\rho(T,P)/\rho(T,P_{ref} = 0.1$ MPa or $P_{sat})$, were compiled from the literature and evaluated using the Tait equation.

Sources of Data

The original experimental data (5703 data points) processed were extracted from the database employed previously for 1-alkanols and *n*-alkanes to which some data obtained from the database installed at Kyoto Institute of Technology have been appended. A list of substances is presented in Table 1 along with Chemical Abstracts 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 members of several classes of C,H,O 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. A significantly lower number of direct experimental data sets, compared to 1-alkanols and *n*-alkanes, was found in the literature. Therefore 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 authors, were included for some substances if no direct experimental (D) or smoothed values (S) were available in the papers. There are some data sets ([73-erm/bai], [75-gus/abd], [76-gus/sad], [77-abd/gus], [77-gus/sad], [78-gus/asl], [78-gus/asl-1], [79-bas/erm]) referenced in the journals of the former Soviet Union as being deposited in VINITI; due to difficulties in obtaining them these deposited data were not included in the evaluation.

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 *n*-alkanes, 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

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

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

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

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

name (alternative name)	CASRN	formula
Ethers		
3-oxapentane (diethyl ether)	60-29-7	$C_4H_{10}O$
4-oxaheptane (di-*n*-propyl ether)	111-43-3	$C_6H_{14}O$
2,4-dimethyl-3-oxapentane (diisopropyl ether)	108-20-3	$C_6H_{14}O$
5-oxanonane (di-*n*-butyl ether)	142-96-1	$C_8H_{18}O$
6-oxaundecane (di-*n*-pentyl ether)	693-65-2	$C_{10}H_{22}O$
8-oxapentadecane (di-*n*-heptyl ether)	629-64-1	$C_{14}H_{30}O$
3,3-dimethyl-2-oxabutane (methyl *tert*-butyl ether)	1634-04-4	$C_5H_{12}O$
4,4-dimethyl-3-oxapentane (ethyl *tert*-butyl ether)	637-92-3	$C_6H_{14}O$
3,3-dimethyl-2-oxapentane (methyl *tert*-pentyl ether)	994-05-8	$C_6H_{14}O$
2,5-dioxahexane (ethylene glycol dimethyl ether)	110-71-4	$C_4H_{10}O_2$
2,5,8-trioxanonane (diethylene glycol dimethyl ether)	111-96-6	$C_6H_{14}O_3$
4,7,10-trioxatridecane (diethylene glycol dipropyl ether)	72072-32-3	$C_{10}H_{22}O_3$
2,5,8,11,14-pentaoxapentadecane (tetraethylene glycol dimethyl ether)	143-24-8	$C_{10}H_{22}O_5$
4-oxa-1,6-heptadiene (diallyl ether)	557-40-4	$C_6H_{10}O$
methoxybenzene (methyl phenyl ether)	100-66-3	C_7H_8O
tetrahydrofuran (oxolane)	109-99-9	C_4H_8O
1,3-dioxolane	646-06-0	$C_3H_6O_2$
tetrahydropyran (oxane)	142-68-7	$C_5H_{10}O$
1,4-dioxane	123-91-1	$C_4H_8O_2$
furan	110-00-9	C_4H_4O
dibenzofuran	132-64-9	$C_{12}H_8O$
Ketones		
2-propanone (dimethyl ketone)	67-64-1	C_3H_6O
2-butanone (methyl ethyl ketone)	78-93-3	C_4H_8O
2-pentanone (methyl *n*-propyl ketone)	107-87-9	$C_5H_{10}O$
3-pentanone (diethyl ketone)	96-22-0	$C_5H_{10}O$
2-hexanone (methyl *n*-butyl ketone)	591-78-6	$C_6H_{12}O$
4-methyl-2-pentanone (methyl isobutyl ketone)	108-10-1	$C_6H_{12}O$
4-heptanone (di-*n*-propyl ketone)	123-19-3	$C_7H_{14}O$
2-octanone (methyl *n*-hexyl ketone)	111-13-7	$C_8H_{16}O$
cyclopentanone	120-92-3	C_5H_8O
cyclohexanone	108-94-1	$C_6H_{10}O$
Aldehydes		
ethanal (acetaldehyde)	75-07-0	C_2H_4O
propanal (propionaldehyde)	123-38-6	C_3H_6O
butanal (butyraldehyde)	123-72-8	C_4H_8O
2-methylpropanal (isobutyraldehyde)	78-84-2	C_4H_8O
pentanal (valeraldehyde)	110-62-3	$C_5H_{10}O$
3-methylbutanal (isovaleraldehyde)	590-86-3	$C_5H_{10}O$
heptanal (enanthaldehyde)	111-71-7	$C_7H_{14}O$
octanal (caprylic aldehyde)	124-13-0	$C_8H_{16}O$
benzaldehyde	100-52-7	C_7H_6O
Acids		
methanoic acid (formic acid)	64-18-6	CH_2O_2
ethanoic acid (acetic acid)	64-19-7	$C_2H_4O_2$
propanoic acid (propionic acid)	79-09-4	$C_3H_6O_2$
2-methylpropanoic acid (isobutyric acid)	79-31-2	$C_4H_8O_2$
octanoic acid (caprylic acid)	124-07-2	$C_8H_{16}O_2$
decanoic acid (capric acid)	334-48-5	$C_{10}H_{20}O_2$
dodecanoic acid (lauric acid)	143-07-7	$C_{12}H_{24}O_2$
tetradecanoic acid (myristic acid)	544-63-8	$C_{14}H_{28}O_2$
hexadecanoic acid (palmitic acid)	57-10-3	$C_{16}H_{32}O_2$
Esters		
methyl ethanoate (methyl acetate)	79-20-9	$C_3H_6O_2$
ethyl ethanoate (ethyl acetate)	141-78-6	$C_4H_8O_2$
1-methylethyl ethanoate (isopropyl acetate)	108-21-4	$C_5H_{10}O_2$
1,2,3-propanetriyl triethanoate (glyceryl triacetate; triacetin)	102-76-1	$C_9H_{14}O_6$
propyl propanoate (*n*-propyl propionate)	106-36-5	$C_6H_{12}O_2$
3-methylbutyl propanoate (isopentyl propionate)	105-68-0	$C_8H_{16}O_2$
methyl hexanoate (methyl caproate)	106-70-7	$C_7H_{14}O_2$
nonyl hexanoate (*n*-nonyl caproate)	101452-99-7	$C_{15}H_{30}O_2$
1,2,3-propanetriyl trihexanoate (glyceryl trihexanoate, tricaproin)	621-70-5	$C_{21}H_{38}O_6$
2-methylpropyl 2-hydroxypropanoate (isobutyl lactate)	61597-96-4	$C_7H_{14}O_3$
pentyl 2-hydroxypropanoate (*n*-pentyl lactate)	6382-06-5	$C_8H_{16}O_3$
methyl benzenecarboxylate (methyl benzoate)	93-58-3	$C_8H_8O_2$
2-ethylhexyl benzenecarboxylate (2-ethylhexyl benzoate)	5444-75-7	$C_{15}H_{22}O_2$
methyl 2-hydroxybenzenecarboxylate (methyl salicylate)	119-36-8	$C_8H_8O_3$
pentyl 2-hydroxybenzenecarboxylate (*n*-pentyl salicylate)	2050-08-0	$C_{12}H_{16}O_3$
hexyl 2-hydroxybenzenecarboxylate (*n*-hexyl salicylate)	6259-76-3	$C_{13}H_{18}O_3$
methyl 2-methyl-2-propenoate (methyl methacrylate)	80-62-6	$C_5H_8O_2$
nonyl 2-methyl-2-propenoate (*n*-nonyl methacrylate)	2696-43-7	$C_{13}H_{24}O_2$
methyl (*Z*)-9-octadecenoate (methyl oleate)	112-62-9	$C_{19}H_{36}O_2$
diethyl 2,2-bis(phenylmethyl)propane-1,3-dioate (diethyl dibenzylmalonate)	597-55-7	$C_{21}H_{24}O_4$

Table 1 (Continued)

name (alternative name)	CASRN	formula
diethyl butane-1,4-dioate (diethyl succinate)	123-25-1	$C_8H_{14}O_4$
dipropyl butane-1,4-dioate (di-*n*-propyl succinate)	925-15-5	$C_{10}H_{18}O_4$
dinonyl butane-1,4-dioate (di-*n*-nonyl succinate)	15805-77-3	$C_{22}H_{42}O_4$
dibutyl benzene-1,2-dicarboxylate (di-*n*-butyl phthalate)	84-74-2	$C_{16}H_{22}O_4$
4-methyl-1,3-dioxolan-2-one (propylene carbonate)	108-32-7	$C_4H_6O_3$

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 the 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 the 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 1,3-dioxolane where only one experimental compressed-liquid data point was available) along with some statistical information of the fits defined as follows:

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

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

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

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

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

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 the figures (Figure 1) which provide 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 the text below.

Table 4 summarizes some statistical information derived from the fits. Only those 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 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 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 the 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 (e.g., 2-butanone; see Table 4) and the enlargement did not result in a distortion of the $B(T)$ function.

As in our previous paper [96-cib/hne] the absence of extremes and inflection points on the function $B(T)$ (eq 3) of all final fits was checked. For 8-oxapentadecane the inflection point was found at the temperature 529 K, which is close to the upper temperature limit of the fit (553 K).

Unlike with 1-alkanols and *n*-alkanes, where a rather large number of sets was available for nearly all selected members of the two homologous series ([94-cib/zik], [96-cib/hne]), the data for the C,H,O compounds considered are,

with few exceptions, scarce (see Table 2). This makes both the critical evaluation and the selection of recommended values rather difficult. The final fits presented in Table 3 should be regarded as smoothed representations of data from one or two sources in many cases. 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 with available independent values published in the literature can be a guide to estimate the reliability of the $P-\rho-T$ data. The values at atmospheric pressure were selected for the comparison presented in Table 5 since the compressibility values published for elevated pressures are usually evaluated from $P-\rho-T$ data and thus they are not independent of data used in the correlations. 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

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

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 5. A substantial part of the speed of sound data used was obtained from the TRC Source Database (Thermodynamics Research Center, College Station, TX). It is obvious from Table 5 that the scatter of isothermal compressibilities taken from the literature is rather large: the average deviation between literature values from different sources is 2.6%; the maximum one is 8%. Outstanding values of deviations, $\delta\beta_T$, obtained from the comparison given in Table 5 may, however, indicate significant inconsistency.

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

Ethers. Surprisingly, no sufficiently accurate data were found for 3-oxapentane (diethyl ether), the substance widely used in any branch of chemistry. The only two sets which are in relatively reasonable mutual agreement (within 2 kg·m^{-3}) are those indicated as retained in Table 4 ([31-bri], [69-bra/fre]). The results of Brazier and Freeman [69-bra/fre] for *n*-alkanes were mostly rejected in previous evaluation (see 96-cib/hne). On the other hand, the isothermal compressibilities calculated from the fit in Table 3 differ from literature values by about 4% on average (see Table 5). The need for new precise $P-\rho-T$ measurements for this common substance is, however, obvious.

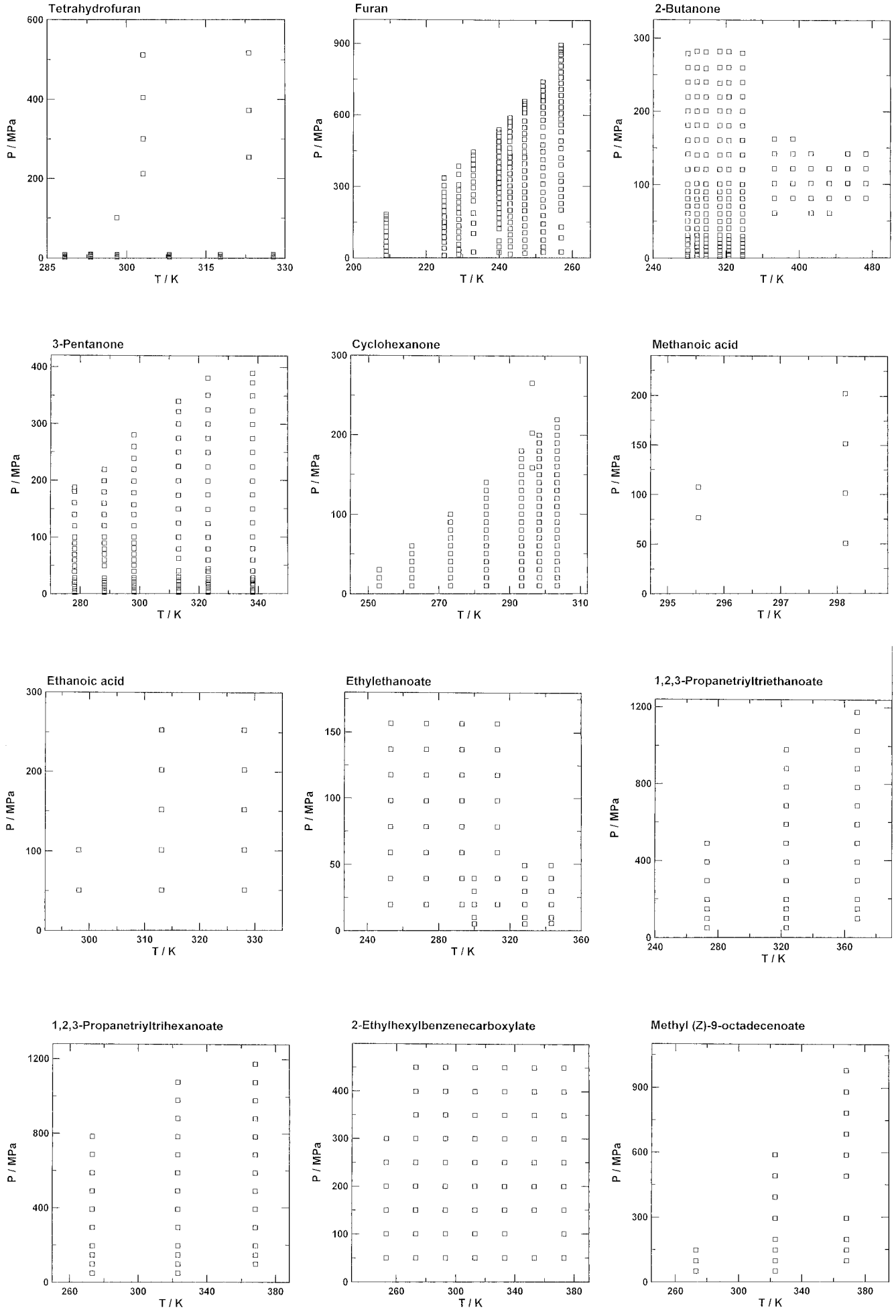
Data for 4-oxaheptane (di-*n*-propyl ether) reported by Safarov et al. [92-saf/mad-1] for larger temperature intervals seem to be slightly less precise than the values given by Skinner et al. [68-ski/cus] for one isotherm with a precision of 1 kg·m^{-3}. However, the Safarov values for 3-oxapentane are, on average (see bias in Table 4), lower than those by Skinner et al. The situation for 4-oxaheptane is the opposite and thus it is difficult to attribute a systematic error to any of the sets. The fit in Table 3 corresponds to Safarov's data covering a broader temperature range, the calculated isothermal compressibility at $P = 0.1$ MPa differs, however, significantly from a value taken from the literature (Table 5). The fit of eq 1 to Skinner's data alone resulted in $c_0 = 0.084\,590$, $b_0 = 57.6582$ MPa, $T_{min} = T_{max} = 303.15$ K, $P_{max} = 499.53$ MPa, RMSD = 0.680 kg·m^{-3}, RMSD$_r$ = 0.083%, bias = 0.055 kg·m^{-3}, $N_p = 10$, and $\pm = 4$. The isothermal compressibility calculated from this fit, β_T(303.15 K, 0.1 MPa) = (1.46 ± 0.03) GPa^{-1}, which is, however, between the literature values for $T = 298.15$ K (see Table 5), seems to be more reasonable than that calculated from Safarov's data [92-saf/mad-1].

In the case of 2,4-dimethyl-3-oxapentane (diisopropyl ether) the deviations of the magnitude in the range from 1.6 to 2.0 kg·m^{-3} were observed for the data measured by Govender et al. [96-gov/let] at $T = 308.15$ K when the original experimental value of reference density, $\rho_{ref}(T = 308.15$ K, $P = 0.1$ MPa) = 708.28 kg·m^{-3}, was used. After this value was replaced by that obtained from the smoothing equation reported by the authors, $\rho_{ref}(T = 308.15$ K, $P = 0.1$ MPa) = 709.83 kg·m^{-3}, the deviations along the isotherm $T = 308.15$ K decreased to the average value 0.22 kg·m^{-3}. The experimental density at $T = 308.15$ K and $P = 0.1$ MPa was also rejected when the data were fit for $P = 0.1$ MPa (Appendix II) due to a large deviation (−1.3 kg·m^{-3}) from a smooth curve. Therefore, the smoothed reference density value 709.83 kg·m^{-3} at $T = 308.15$ K was used for the final fit (Table 3). The thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$, at $T = 298.15$ K and $P = 0.1$ MPa evaluated from the fit in Appendix II is, however, significantly lower (1.17 kK^{-1}) than the value by Obama et al. [85-oba/ood] (1.45 kK^{-1}); this disagreement is similar to that observed for data for other ethers reported by Govender et al. [96-gov/let] (see below). Compressed-liquid density data reported by Schornack and Eckert [70-sch/eck] seem to be inconsistent with the original reference values (at $P = 0.1$ MPa) and thus the values at lower pressures were rejected while those at the high pressure range were retained since the effect on the fit of data at the low pressure range ([96-gov/let]) was negligible.

There was only one $P-\rho-T$ data set available for 5-oxanonane (di-*n*-butyl ether). The agreement of isothermal compressibility calculated from the fit with the value taken from the literature is −1.1% (Table 5), indicating a reliability of data measured by Senger [94-sen], which is evident also in the case of 2,5,8-trioxanonane (deviation in isothermal compressibility below 1%).

The two data sets available for 6-oxaundecane (di-*n*-pentyl ether) agree within the experimental error in the range of lower pressures but deviations above 10 kg·m^{-3} were observed for Bridgman's [49-bri] values at high pressures. Since the experimental temperature of Bridgman's measurements is uncertain (room temperature reported to be about 298 K) and data at high pressures were obtained using a lead capsule to separate the sample from a hydraulic fluid, his all high-pressure data were rejected. On the other hand, all values reported by Safarov et al. [92-saf/mad] for the isobar 19.62 MPa were also rejected due to large negative deviations (−4.8 kg·m^{-3} in an average) from a smooth fit, indicating an erroneous pressure value. Besides that, an obvious typographical error in Safarov's data was corrected; the original value $\rho(T = 414.36$ K, $P = 0.101$ MPa) = 579.2 kg·m^{-3} was replaced by 679.2 kg·m^{-3}. The deviation between the calculated and literature value of isothermal compressibility at $P = 0.1$ MPa is rather large (−14%; see Table 5).

The only data set available for 8-oxapentadecane (di-*n*-heptyl ether, [93-saf/oso]) seems to be internally inconsistent since large deviations (10 kg·m^{-3} in an average) were observed at pressures below 19.6 MPa, indicating an inconsistency of compressed liquid data with densities reported for atmospheric pressure. This may be the reason why the inflection point appeared on the *B(T)* curve, as mentioned above. Similarly, the values for 4-oxa-1,6-heptadiene reported by Safarov et al. [92-saf/gus] for pressure $P = 9.81$ MPa were rejected due to large deviations (about 4 kg·m^{-3} in an average).


Tetrahydrofuran
Furan
2-Butanone
3-Pentanone
Cyclohexanone
Methanoic acid
Ethanoic acid
Ethylethanoate
1,2,3-Propanetriyltriethanoate
1,2,3-Propanetriyltrihexanoate
2-Ethylhexylbenzenecarboxylate
Methyl (Z)-9-octadecenoate
P / MPa
T / K

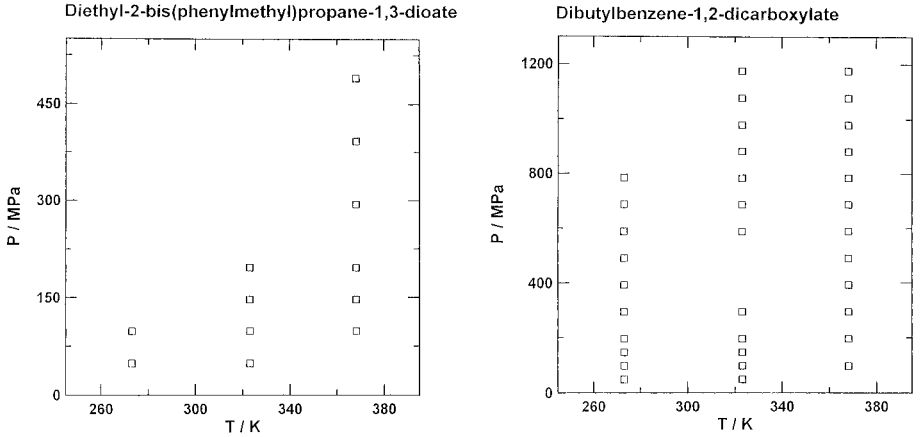


Figure 1. Temperature and pressure coordinates of data points retained in the correlations for the fits where $T-P$ areas of retained data points are not rectangular.

The deviations between the two data sets available for 2,5-dioxahexane (ethylene glycol dimethyl ether) exceed experimental uncertainties declared by the authors (0.3 kg·m^{-3} [94-sen], 0.4 kg·m^{-3} [78-sha/bai]) in the common temperature range. The fit in Table 3 corresponds to values by Senger [94-sen] over a much larger pressure range than that reported by Sharipov and Bairamova [78-sha/bai] which, being correlated alone, resulted in (the maximum temperature of original smoothed reference densities was 330 K, see Appendix I) $c_0 = 0.272\,862$, $b_0 = 299.2118$ MPa, $b_1 = -225.3534$ MPa·K^{-1}, $T_0 = 298.15$ K, $T_{min} = 298.15$ K, $T_{max} = 323.15$ K, $P_{max} = 35.91$ MPa, RMSD = 0.386 kg·m^{-3}, RMSD$_r$ = 0.046%, bias = −0.107 kg·m^{-3}, $N_p = 12$, $\pm = 0$. The isothermal compressibility, $\beta_T(T = 303.15$ K, $P = 0.1$ MPa), calculated from this fit differs from that calculated from the fit in Table 3 by −18%. The parameter c_0 (and of b_i as well) of this fit has a value unusually high for the Tait equation. Similarly high values were obtained for 4,7,10-trioxatridecane (diethylene glycol dipropyl ether; see Table 3) for the fit of data from the same laboratory [81-sha/abd].

Senger [94-sen] measured $P-\rho-T$ data for several ethers using a bellows piezometer and presented all the experimental values along each isotherm on the increase of pressure up to the maximum one and then on the decrease to a low pressure range. A hysteresis was observed when correlating his data for 3,3-dimethyl-2-oxabutane (methyl *tert*-butyl ether) and 4,4-dimethyl-3-oxapentane (ethyl *tert*-butyl ether); the deviations from the eq 1 were negative for the pressure-on-increase data points and positive for decreasing pressure. The hysteresis resulted in rather higher values of RMSD for these two ethers compared to those measured by Senger for other ethers where the hysteresis was much less pronounced. The effect seems to be symmetrical since the values of bias for all ethers are comparable. The agreement of relative densities, $\rho(T,P)/\rho(T,P_{ref} = 0.1$ MPa) reported by Senger [94-sen] and Govender et al. [96-gov/let] for 3,3-dimethyl-2-oxabutane (methyl *tert*-butyl ether) and 3,3-dimethyl-2-oxapentane (methyl *tert*-pentyl ether) is satisfactory (see Table 4). Large discrepancies were, however, observed for reference values (densities at $P = 0.1$ MPa) where maximum deviations between the two sets were as high as 10 kg·m^{-3}; the data [96-gov/let] yield lower values of thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$, than other sources (see also discussion for cyclic ethers below). At $T = 298.15$ K and $P = 0.1$ MPa the values of α_P for 3,3-dimethyl-2-oxabutane and 3,3-dimethyl-2-oxapentane are $\alpha_P = 1.11$ kK^{-1} [96-gov/let], 1.47 kK^{-1} [94-sen], 1.42 kK^{-1} [85-oba/ood], and $\alpha_P = 0.96$ kK^{-1} [96-gov/let], 1.25 kK^{-1} [94-sen], respectively. Senger's values of α_P are in good agreement with the literature data also for 4,4-dimethyl-3-oxapentane (ethyl *tert*-butyl ether); $\alpha_P(T = 298.15$ K, $P = 0.1$ MPa) = 1.45 kK^{-1} [94-sen], 1.40 kK^{-1} [85-oba/ood]. Since Senger's values are not currently available and are in better agreement with other literature data, the fits of data at $P = 0.1$ MPa by Senger [94-sen] are presented in Appendix II; the values reported by Govender et al. [96-gov/let] are easily available from the original source.

Similarly as for 4-oxaheptane, the negative deviations of values reported by Skinner et al. [68-ski/cus] for methoxybenzene from the data measured by Kuss and Taslimi [70-kus/tas] were observed. The final fit corresponds to the latter data set; the fit of Skinner's data resulted in $c_0 = 0.081\,446$, $b_0 = 125.8382$ MPa, $T_{min} = T_{max} = 303.15$ K, $P_{max} = 497.51$ MPa, RMSD = 1.808 kg·m^{-3}, RMSD$_r$ = 0.166%, bias = 0.022 kg·m^{-3}, $N_p = 10$, $\pm = 0$. The isothermal compressibility, $\beta_T(T = 303.15$ K, $P = 0.1$ MPa), calculated from this fit differs from that calculated from the fit in Table 3 by −4.2%.

The $P-\rho-T$ data for cyclic ethers are scarce. One experimental value was found for 1,3-dioxolane ([83-nak/miy]; $\{\rho(P = 101.3$ MPa)/$\rho(P = 0.1$ MPa) − 1$\} = 0.055\,39$ at $T = 298.15$ K), and therefore no correlation was performed. Data for tetrahydrofuran reported by Schornack and Eckert [70-sch/eck] are of low accuracy and show an internal inconsistency, particularly at lower pressures. The data at higher pressures were, however, retained in the final fit to enlarge the pressure range. Two values presented for 1,4-dioxane in reference 68-pea/str for $T = 298.15$ K are reasonably consistent with the data measured by Govender et al. [96-gov/let] in the lower pressure range. The rejected value reported by Korpela and Koskikallio [66-kor/kos] for $T = 298.15$ K and $P = 67.3$ MPa differs from the final fit (Table 3) by 5.4 kg·m^{-3}. Deviations of isothermal compressibilities, $\beta_T(T,P = 0.1$ MPa), calculated from the fits presented for tetrahydrofuran and 1,4-dioxane in Table 3 from the values obtained from the literature data are below 6 and 8%, respectively, except for those cases where density and thermal expansivity used in eq 11 were evaluated from the $\rho(T,P = 0.1$ MPa) data by Govender at al. [96-gov/let] (see Table 5). Similarly as in the case of 2,4-dimethyl-3-oxapentane, 3,3-dimethyl-2-oxabutane, and 3,3-dimethyl-2-oxapentane (see above), large deviations of the $\rho(T,P = 0.1$ MPa) values [96-gov/let] from other available data were observed, resulting in significantly lower values of thermal expansivity, α_P. Therefore the values of isothermal compressibility, β_T, calculated from eq 11 using the $\rho(T,P = 0.1$ MPa) data by Govender at al. [96-gov/let] are lower (compared to other literature values in Table 5) and not consistent even with relative densities, $\rho(T,P)/\rho(T,P_{ref} = 0.1$ MPa) reported in 96-gov/let; the values

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] %
				3-Oxapentane (Diethyl Ether)				
13-bri	119	293.15	353.15	49.0	1176.8	vs	D	
31-bri	26	303.15	348.15	49.1	1176.9	vb	D	
57-wal/ric	2	294.15	305.15	4180.0	9610.0	sw	D	
68-ski/cus	11	303.15	303.15	82.1	500.6	vl	D	
69-bra/fre	8	303.15	303.15	50.0	400.0	vb	D	
92-saf/mad	88	296.71	462.18	4.9	98.1	bu	D	
total	254	293.15	462.18	4.9	9610.0			
				4-Oxaheptane (Di-*n*-propyl Ether)				
68-ski/cus	11	303.15	303.15	49.7	499.5	vl	D	
92-saf/mad-1	110	294.30	524.80	4.9	98.1	bu	D	
total	121	294.30	524.80	4.9	499.5			
				2,4-Dimethyl-3-oxapentane (Diisopropyl Ether)				
70-sch/eck	12	303.15	323.15	45.7	511.3	vb	D	
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	99.8m[e]
total	57	288.15	328.15	0.5	511.3			
				5-Oxanonane (Di-*n*-butyl Ether)				
94-sen	90	298.15	328.15	5.1	203.7	vb	D	99[d]
				6-Oxaundecane (Di-*n*-pentyl Ether)				
49-bri	11	298.15	298.15	49.0	980.7	vs	D	
92-saf/mad	132	296.64	561.57	4.9	98.1	bu	D	
total	143	296.64	561.57	4.9	980.7			
				8-Oxapentadecane (Di-*n*-heptyl Ether)				
93-saf/oso	154	293.00	553.00	4.9	98.1	bu	D	
				3,3-Dimethyl-2-oxabutane (Methyl *tert*-Butyl Ether)				
94-sen	90	298.15	328.15	5.4	207.7	vb	D	99[d]
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	>99.9m[e]
total	135	288.15	328.15	0.5	207.7			
				4,4-Dimethyl-3-oxapentane (Ethyl *tert*-Butyl Ether)				
94-sen	90	298.15	328.15	5.6	207.2	vb	D	>99[d]
				3,3-Dimethyl-2-oxapentane (Methyl *tert*-Pentyl Ether)				
94-sen	90	298.15	328.15	5.6	203.8	vb	D	98[d]
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	>99.9m[e]
total	135	288.15	328.15	0.5	203.8			
				2,5-Dioxahexane (Ethylene Glycol Dimethyl Ether)				
78-sha/bai	48	298.15	473.15	1.8	36.6	pi	D	99.94w[e]
94-sen	90	298.15	328.15	5.6	204.8	vb	D	99[d]
total	138	298.15	473.15	1.8	204.8			
				2,5,8-Trioxanonane (Diethylene Glycol Dimethyl Ether)				
94-sen	90	298.15	328.15	5.1	202.8	vb	D	99[d]
				4,7,10-Trioxatridecane (Diethylene Glycol Dipropyl Ether)				
81-sha/abd	69	298.15	523.15	2.2	35.9	pi	D	
				2,5,8,11,14-Pentaoxapentadecane (Tetraethylene Glycol Dimethyl Ether)				
90-sve/sid	5	293.15	293.15	2.0	10.0	mo	D[f]	99.5[e]
				4-Oxa-1,6-heptadiene (Diallyl Ether)				
92-saf/gus	121	291.70	552.30	4.9	99.1	bu	D	
				Methoxybenzene (Methyl Phenyl Ether)				
68-ski/cus	10	303.15	303.15	59.3	497.5	vl	D	
70-kus/tas	20	298.15	353.15	39.2	196.1	vl	D	
total	30	298.15	353.15	39.2	497.5			
				Tetrahydrofuran (Oxolane)				
70-sch/eck	12	303.15	323.15	46.7	517.0	vb	D	
71-ham/smi	1	303.15	303.15	101.3	101.3	va	D	99[d]
83-nak/miy	1	298.15	298.15	101.3	101.3	va	D	
87-hol/goe	5	293.15	293.15	2.0	10.0	mo	D[f]	>99[d]
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	>99.9m[e]
total	64	288.15	328.15	0.5	517.0			
				1,3-Dioxolane				
83-nak/miy	1	298.15	298.15	101.3	101.3	va	D	
				Tetrahydropyran (Oxane)				
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	>99.9m[e]

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] %
				1,4-Dioxane				
66-kor/kos	1	298.15	298.15	67.3	67.3	va	D	
68-pea/str	2	298.15	298.15	25.0	50.0	va	S	
96-gov/let	45	288.15	328.15	0.5	8.0	mo	D[f]	>99.9m[e]
total	48	288.15	328.15	0.5	67.3			
				Furan				
78-fig/szw	191	209.00	257.00	11.0	897.0	vb	D	>99[e]
				Dibenzofuran				
84-nas/siv	42	391.55	563.15	0.5	25.5	vs	D	99.99m[e]
				2-Propanone (Dimethyl Ketone)				
13-bri	109	293.15	353.15	49.0	1176.8	vs	D	
51-new/wea	1	298.15	298.15	101.3	101.3	va	D	
56-stu	1	303.15	303.15	101.3	101.3	va	D	
57-wal/ric	2	299.15	303.15	4640.0	10580.0	sw	D	
66-win/pow	4	273.15	273.15	34.5	206.8	vb	F	
66-win/pow	4	273.15	273.15	34.5	206.8	vb	F	
66-win/pow	9	273.15	273.15	34.5	586.1	vb	F	
67-ada/lai	7	299.76	299.76	40.0	100.0	vs	D	
76-ato/mam	48	273.15	473.15	20.3	162.1	hp	D	
77-gup/han	24	273.15	363.15	2.8	22.1	vs	D	
80-rae/fin	49	298.15	398.15	1.0	411.9	vb	D	
87-hol/goe-1	5	293.15	293.15	2.0	10.0	mo	D[f]	>99.8m[e]
87-nhu/bha	5	293.15	293.15	2.0	10.0	mo	D	99.99[e]
91-mal/woo	105	278.15	323.15	2.5	392.3	vb	D	99.9m[d]
91-pap/zia	9	298.15	298.15	2.0	33.8	mo	D	99.5[d]
92-ego/gru	5	298.15	298.15	5.0	60.0	va	D	
total	387	273.15	473.15	1.0	10580.0			
				2-Butanone (Methyl Ethyl Ketone)				
63-and	9	283.15	308.15	167.9	305.1	va	F	
74-ato/mam	243	283.15	473.15	9.8	127.5	hp	D	
76-ato/bag	77	273.15	473.15	40.5	162.1	hp	D	
77-lam/hun	15	303.15	343.15	35.0	172.0	vs	D	
92-mal/woo	138	278.15	338.15	2.3	282.5	vb	D	>99.9m[d]
total	482	273.15	473.15	2.3	305.1			
				2-Pentanone (Methyl *n*-Propyl Ketone)				
77-apa/ker	36	273.00	472.24	5.0	78.6	bu	D	99.86[e]
				3-Pentanone (Diethyl Ketone)				
82-ato/mam	90	293.00	473.00	9.8	156.8	hp	D	
93-mal/pri	128	278.15	338.15	2.5	389.8	vb	D	>99.0m[d]
total	218	278.15	473.00	2.5	389.8			
				2-Hexanone (Methyl *n*-Butyl Ketone)				
79-ato	90	293.15	473.15	9.8	156.9	hp	D	
				4-Methyl-2-pentanone (Methyl Isobutyl Ketone)				
63-and	13	295.55	295.55	245.2	484.8	va	D	
				4-Heptanone (Di-*n*-propyl Ketone)				
91-ato	108	273.00	473.00	10.0	160.0	hp	D	
				2-Octanone (Methyl *n*-Hexyl Ketone)				
75-ato/mam	88	273.15	473.15	20.3	162.1	bu	D	
78-apa/ker	44	273.15	566.08	5.0	78.6	bu	D	
total	132	273.15	566.08	5.0	162.1			
				Cyclopentanone				
69-bra/fre	8	298.15	298.15	50.0	400.0	vb	D	
				Cyclohexanone				
63-and	3	296.45	296.45	158.7	266.1	va	F	
82-wis/wue	93	253.20	303.40	10.0	220.0	vs	S	99.9[e]
total	96	253.20	303.40	10.0	266.1			
				Ethanal (Acetaldehyde)				
68-cha/sta	10	295.15	295.15	13.9	138.0	vs	D	
				Propanal (Propionaldehyde)				
68-cha/sta	10	296.65	296.65	13.9	138.0	vs	D	
				Butanal (Butyraldehyde)				
68-cha/sta	10	302.04	302.04	13.9	138.0	vs	D	
71-run/sta	32	303.15	333.15	34.9	276.6	vs	D	
total	42	302.04	333.15	13.9	276.6			
				2-Methylpropanal (Isobutyraldehyde)				
68-cha/sta	10	301.37	301.37	13.9	138.0	vs	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] %
				Pentanal (Valeraldehyde)				
75-mam/gus	48	248.15	545.15	5.0	50.1	bu	D	99.8m[d]
				3-Methylbutanal (Isovaleraldehyde)				
68-cha/sta	10	300.37	300.37	13.9	138.0	vs	D	
75-mam/gus	52	284.95	580.36	5.0	50.1	bu	D	>99.8m[d]
total	62	284.95	580.36	5.0	138.0			
				Heptanal (Enanthaldehyde)				
68-cha/sta	10	295.21	295.21	13.9	138.0	vs	D	
				Octanal (Caprylic Aldehyde)				
68-cha/sta	10	293.87	293.87	13.9	138.0	vs	D	
				Benzaldehyde				
68-cha/sta	10	295.21	295.21	13.9	138.0	vs	D	
				Methanoic Acid (Formic Acid)				
63-and	2	295.55	295.55	76.5	107.5	va	F	98[d]
71-kor	4	298.15	298.15	50.7	202.7	va	F	
total	6	295.55	298.15	50.7	202.7			
				Ethanoic Acid (Acetic Acid)				
71-kor	12	298.15	328.15	50.7	253.3	va	F	
				Propanoic Acid (Propionic Acid)				
71-kor	15	298.15	328.15	50.7	253.3	va	F	
				2-Methylpropanoic Acid (Isobutyric Acid)				
71-kor	15	298.15	328.15	50.7	253.3	va	F	99.8[e]
				Octanoic Acid (Caprylic Acid)				
92-ban/gar	30	343.15	373.15	1.0	9.0	mo	D[f]	>99.5m[d]
				Decanoic Acid (Capric Acid)				
92-ban/gar	30	343.15	373.15	1.0	9.0	mo	D[f]	>99m[d]
				Dodecanoic Acid (Lauric Acid)				
92-ban/gar	30	343.15	373.15	1.0	9.0	mo	D[f]	>99.5m[d]
				Tetradecanoic Acid (Myristic Acid)				
92-ban/gar	25	353.15	373.15	1.0	9.0	mo	D[f]	>99.5m[d]
				Hexadecanoic Acid (Palmitic Acid)				
92-ban/gar	25	353.15	373.15	1.0	9.0	mo	D[f]	>99m[d]
				Methyl Ethanoate (Methyl Acetate)				
78-kum/iwa	32	253.15	313.15	19.7	156.8	vl	D	97.0[d]
				Ethyl Ethanoate (Ethyl Acetate)				
49-bri	17	298.15	298.15	49.0	3922.7	vs	D	
63-and	1	298.15	298.15	466.1	466.1	va	S	
70-sch/eck	12	303.15	323.15	51.5	512.7	vb	D	
75-gus/kad	42	300.06	499.21	5.0	49.1	bu	D	99.8[e]
79-kum/iwa	32	253.15	313.15	19.7	156.8	vl	D	99[d]
total	104	253.15	499.21	5.0	3922.7			
				1-Methylethyl Ethanoate (Isopropyl Acetate)				
75-gus/kad	48	297.17	531.22	5.0	49.1	bu	D	99.8[e]
				1,2,3-Propanetriyl Triethanoate (Glyceryl Triacetate; Triacetin)				
32-bri	32	273.15	368.15	49.0	1176.8	vb	D	
				Propyl Propanoate (*n*-Propyl Propionate)				
78-gus/kli	66	300.00	550.00	5.0	50.0	bu	S	99.8w[e]
				3-Methylbutyl Propanoate (Isopentyl Propionate)				
76-gus/kli	78	298.15	598.15	5.0	50.1	bu	S	99.7[e]
				Methyl Hexanoate (Methyl Caproate)				
92-mus/gus	90	294.99	589.63	4.9	58.8	bu	D	99.88[e]
				Nonyl Hexanoate (*n*-Nonyl Caproate)				
92-mus/gus-1	119	289.00	604.82	4.9	58.8	bu	D	99.32[e]
				1,2,3-Propanetriyl Trihexanoate (Glyceryl Trihexanoate; Tricaproin)				
32-bri	36	273.15	368.15	49.0	1176.8	vb	D	
				2-Methylpropyl 2-Hydroxypropanoate (Isobutyl Lactate)				
91-gus/kul	121	294.36	533.89	4.9	98.1	bu	D	99.68[e]
				Pentyl 2-Hydroxypropanoate (*n*-Pentyl Lactate)				
91-gus/kul-1	121	296.71	535.03	4.9	98.1	bu	D	99.48[e]
				Methyl Benzenecarboxylate (Methyl Benzoate)				
94-mus/tag	105	300.48	604.58	5.0	58.9	bu	D	99.3[e]
				2-Ethylhexyl Benzenecarboxylate (2-Ethylhexyl Benzoate)				
88-wal/lam	60	253.15	373.15	50.0	450.0	nd	D	>99.8[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] %
Methyl 2-Hydroxybenzenecarboxylate (Methyl Salicylate)								
90-mus/gan-1[g]	72	298.15	573.15	10.0	60.0	bu	D	99.7[e]
Pentyl 2-Hydroxybenzenecarboxylate (*n*-Pentyl Salicylate)								
90-mus/gan-1	72	298.15	573.15	10.0	60.0	bu	D	99.7[e]
Hexyl 2-Hydroxybenzenecarboxylate (*n*-Hexyl Salicylate)								
90-mus/gan-1	72	298.15	573.15	10.0	60.0	bu	D	99.7[e]
Methyl 2-Methyl-2-propenoate (Methyl Methacrylate)								
87-gus/bai	142	289.34	424.77	5.0	98.1	bu	D	99.92[d]
Nonyl 2-Methyl-2-propenoate (*n*-Nonyl Methacrylate)								
89-gus/bai	78	292.37	473.43	5.0	98.2	bu	D	99.94[e,h]
Methyl (*Z*)-9-Octadecenoate (Methyl Oleate)								
32-bri	22	273.15	368.15	49.0	980.7	vb	D	
Diethyl 2,2-Bis(phenylmethyl)-propane-1,3-dioate (Diethyl Dibenzylmalonate)								
32-bri	13	273.15	368.15	49.0	490.3	vb	D	
Diethyl Butane-1,4-dioate (Diethyl Succinate)								
90-mus/gan-3	54	295.65	498.15	5.0	49.1	bu	D	98.6[e]
Dipropyl Butane-1,4-dioate (Di-*n*-propyl Succinate)								
90-mus/gan-2	60	288.15	502.75	5.0	49.1	bu	D	98.7[e]
Dinonyl Butane-1,4-dioate (Di-*n*-nonyl Succinate)								
91-mus/gan	72	298.15	573.15	10.0	60.0	bu	D	99.37[e]
Dibutyl Benzene-1,2-dicarboxylate (Di-*n*-butyl Phthalate)								
32-bri	37	273.15	368.15	49.0	1176.8	vb	D	
4-Methyl-1,3-dioxolan-2-one (Propylene Carbonate)								
92-uos/kit	4	298.15	298.15	50.0	200.0	va	D	

[a] Method used for measurements: bu, buoyancy method; mo, mechanical oscillator method; nd, not described or stated in the reference; pi, piezometer of unspecified 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; F, values calculated from smoothing equation reported by the researchers. [c] No letter, unspecified percent; m, mole percent; w, mass percent. [d] Only purity of source material is given. [e] Final purity of the sample. [f] IPTS-68 declared by the researchers. [g] Same data are presented also in 90-mus/gan. [h] Purified sample was stabilized with 0.05 mass % of hydrochinone to prevent a polymerization.

of β_T(T = 298.15 K, P = 0.1 MPa) evaluated by Govender et al. [96-gov/let] from their data are 0.960 GPa^{-1} (tetrahydrofuran) and 0.739 GPa^{-1} (1,4-dioxane). It might be concluded that while the compression data (relative densities) along the isotherms seem to be correct, the temperature dependencies of density itself need to be reexamined.

There was one data set available for tetrahydropyran [96-gov/let]. The agreement of the value of β_T(T = 298.15 K, P = 0.1 MPa) calculated from the fit with the value selected from the literature is very good (−0.4%, Table 5). Table A2 (Appendix II) presents the fit of data at P = 0.1 MPa; it is likely that the value of the parameter v_1 of the smoothing equation presented in the original source [96-gov/let] is in error; the correct value should be probably 0.076 166 (not 0.761 66), as deduced from tentative calculations of densities at P = 0.1 MPa. Besides that, it should be pointed out that, similarly as with other ethers measured by Govender et al. [96-gov/let], the values of thermal expansivity α_P are significantly lower (e.g., α_P(T = 298.15 K, P = 0.1 MPa) = 0.776 kK^{-1}) than those evaluated from other literature data (83-ing/gro: α_P(T = 298.15 K, P = 0.1 MPa) = 1.15 kK^{-1}).

Data of furan measured by Figuiere and Szwarc [78-fig/szw] are of low accuracy (RMSD = 2.4 kg·m^{-3}); the authors primarily investigated solid−liquid equilibrium and the $P-\rho-T$ measurements were of secondary importance. Experimental data of dibenzofuran [84-nas/siv] correlated by the authors using a modified Chueh equation with 20 parameters resulted in the relative $RMSD_r$ slightly lower (0.07%) than that of the fit by eq 1 with four adjustable parameters (Table 3). It was, however, impossible to improve the fit by additional parameters since the extreme appeared on the $B(T)$ curve.

Ketones (Alkanones and Cyclohexanone). There is a rather large number of data sets available for 2-propanone. The evaluation revealed that only a few data sets measured recently in a close-to-ambient temperature range are in a mutual agreement. It was not possible to extend the temperature range by an inclusion of some less accurate data sets since inflection points appeared on the *B-(T)* curve indicating the inconsistency of data. The extension was possible in the case of 2-butanone by retaining the high-temperature data points from the set of Atoyan et al. [76-ato/bag] but the expected uncertainty in this temperature range might be rather high (RMSD = 2.5 kg·m^{-3}; see Table 4). The agreement between values of β_T(T,P = 0.1 MPa) calculated from the fits for those two alkanones and data taken from the literature is satisfactory (see Table 5), even for 2-butanone at temperatures beyond Malhotra's [92-mal/woo] experimental temperature range.

There is only one data set available for 2-pentanone: a comparison of smoothed values with those from the generalized Tait equation (see below and Table 6) shows a satisfactory agreement (0.16%); however, the isothermal compressibilities (Table 5) calculated from the fit in Table 3 are lower than selected literature values. The data set by Atoyan and Mamedov [82-ato/mam] for 3-pentanone is inconsistent with data measured by Malhotra et al. [93-mal/pri] and since the data from Malhotra's laboratory proved to be of high quality in the case of 2-propanone and 2-butanone, the latter set only was retained.

Data available for 2-hexanone seem to be of poor accuracy. The values of isothermal compressibility calculated from the fit for P = 0.1 MPa differ from the values taken from the literature by nearly −20% at lower temperatures (see Table 5) and are even out of a monotonous decrease within the homologous series of 2-alkanones indicated by the literature data. Besides that, the deviations of relative density from the generalized Tait equation (see below and

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

Ethers

	3-oxa-pentane	4-oxa-heptane	2,4-di-methyl-3-oxapentane	5-oxa-nonane	6-oxa-undecane	8-oxa-penta-decane	3,3-di-methyl-2-oxabutane	4,4-di-methyl-3-oxapentane	3,3-di-methyl-2-oxapentane	2,5-dioxa-hexane
c_0	0.095070	0.085992	0.088836	0.090642	0.133853	0.156481	0.091636	0.086511	0.087240	0.092603
b_0/MPa	46.6780	50.2436	45.5640	74.8969	143.6450	198.1315	52.6240	48.4404	64.0716	83.5587
b_1/MPa·K^{-1}	−43.4590	−38.7232	−55.9497	−47.3687	−103.5338	−153.7136	−41.6220	−35.0754	−49.9481	−65.9447
b_2/MPa·K^{-2}		15.5294	14.5106		27.0944	55.2218	25.9452		13.4133	
b_3/MPa·K^{-3}						−7.8176				
T_0/K	303.15	294.30	303.15	298.15	298.15	293.00	298.15	298.15	298.15	298.15
T_{min}/K	303.15	294.30	288.15	298.15	296.64	293.00	288.15	298.15	288.15	298.15
T_{max}/K	348.15	374.50	328.15	328.15	456.82	553.00	328.15	328.15	328.15	328.15
P_{min}/MPa	49.13	4.91	0.50	5.08	4.91	19.62	0.50	5.56	0.50	5.58
P_{max}/MPa	1176.90	98.10	511.29	203.68	98.10	98.10	207.72	207.16	203.79	204.75
RMSD/kg·m^{-3}	1.220	1.361	1.172	0.233	1.429	1.793	0.765	0.483	0.290	0.225
$RMSD_r$/%	0.138	0.183	0.135	0.029	0.189	0.228	0.095	0.062	0.036	0.025
bias/kg·m^{-3}	−0.098	0.224	0.062	0.020	0.043	−0.095	0.054	0.015	−0.011	0.028
N_p	33	40	52	90	80	113	134	90	135	90
±	−1	6	4	−2	6	−13	−10	0	7	10
s_w	0.957	1.000	1.031	0.955	1.069	1.020	1.066	1.122	1.170	0.920

	2,5,8-tri-oxanonane	4,7,10-tri-oxatridecane	2,5,8,11,14-pentaoxa-pentadecane	4-oxa-1,6-heptadiene	methoxy-benzene	tetra-hydro-furan	tetra-hydro-pyran	1,4-dioxane	furan	dibenzo-furan
c_0	0.089658	0.363718	0.086177	0.185068	0.095902	0.092962	0.055469	0.042888	0.094453	0.017847
b_0/MPa	109.6532	362.4873	137.1726	163.5259	142.0376	87.2488	56.1224	54.3581	123.0858	12.0064
b_1/MPa·K^{-1}	−82.7022	−250.7135		−95.2772	−77.7516	−90.0809	−59.8283	−47.0832	−68.6050	−6.4553
b_2/MPa·K^{-2}	25.4503			50.3120		75.8269	49.5308	33.6213		1.2142
T_0/K	298.15	348.15	293.15	291.70	303.15	303.15	298.15	298.15	257.00	423.15
T_{min}/K	298.15	298.15	293.15	291.70	298.15	288.15	288.15	288.15	209.00	391.55
T_{max}/K	328.15	348.15	293.15	365.00	353.15	328.15	328.15	328.15	257.00	563.15
P_{min}/MPa	5.08	2.18	2.00	4.91	39.23	0.50	0.50	0.50	11.00	0.51
P_{max}/MPa	202.81	35.94	10.00	98.10	196.13	516.96	8.00	50.00	897.00	25.53
RMSD/kg·m^{-3}	0.173	0.392	0.007	1.680	0.158	0.907	0.094	0.273	2.385	1.080
$RMSD_r$/%	0.018	0.045	0.001	0.230	0.015	0.091	0.011	0.026	0.213	0.103
bias/kg·m^{-3}	0.013	−0.114	−0.001	0.140	0.000	−0.027	−0.009	0.024	0.001	0.037
N_p	90	22	5	38	20	58	45	47	185	38
±	8	−6	−1	6	2	16	−5	3	49	−2
s_w	1.040	1.094	0.973	1.030	1.086	1.280	0.991	1.007	0.955	1.324

Ketones and Aldehydes

	2-propanone	2-butanone	2-pentanone	3-pentanone	2-hexanone	4-methyl-2-pentanone	4-heptanone	2-octanone	cyclo-pentanone	cyclo-hexanone
c_0	0.099239	0.095009	0.087406	0.094603	0.085246	0.099088	0.102388	0.113614	0.098473	0.091558
c_1/K^{-1}		−0.003291								
b_0/MPa	80.3063	71.7822	107.5762	90.6753	106.7265	99.9725	150.4746	155.4195	95.7265	135.5573
b_1/MPa·K^{-1}	−75.4324	−62.6158	−87.2636	−69.3353	−106.2848		−121.9168	−103.9260		−52.1027
b_2/MPa·K^{-2}	37.3329	23.6819		19.0573	59.3556		35.0029	17.5846		130.4980
b_3/MPa·K^{-3}		−8.7208			−16.7670					
b_4/MPa·K^{-4}		1.6959								
T_0/K	293.15	313.15	273.00	298.15	293.15	295.55	273.00	273.15	298.15	303.40
T_{min}/K	278.15	278.15	273.00	278.15	293.15	295.55	273.00	273.15	298.15	253.20
T_{max}/K	323.15	473.15	315.66	338.15	393.15	295.55	403.00	374.31	298.15	303.40
P_{min}/MPa	2.00	2.32	5.01	2.53	9.81	245.21	10.00	5.01	50.00	10.00
P_{max}/MPa	392.25	282.45	78.58	389.82	156.91	484.84	160.00	78.58	400.00	266.08
RMSD/kg·m^{-3}	0.266	1.079	0.279	0.307	0.990	0.802	1.102	0.550	5.847	0.699
$RMSD_r$/%	0.032	0.137	0.033	0.036	0.125	0.085	0.129	0.067	0.565	0.071
bias/kg·m^{-3}	0.058	0.003	−0.054	0.087	−0.132	0.029	−0.012	−0.070	−0.318	−0.033
N_p	124	165	18	128	53	13	71	25	8	96
±	26	3	−2	36	3	−3	17	−7	0	8
s_w	1.028	0.931	1.163	1.025	0.921	0.999	1.133	1.006	1.017	1.003

	ethanal	propanal	butanal	2-methylpropanal	pentanal	3-methylbutanal	heptanal	octanal	benzaldehyde
c_0	0.107840	0.120241	0.091785	0.103047	0.071630	0.094111	0.102239	0.102738	0.094041
b_0/MPa	72.5470	110.1100	102.7158	79.8182	74.4381	82.1858	112.9950	121.6201	154.0605
b_1/MPa·K^{-1}			−38.5961		−20.4294	−45.1467			
b_2/MPa·K^{-2}			−97.6281		−12.2063	−19.1201			
T_0/K	295.15	296.65	302.04	301.37	248.15	300.37	295.21	293.87	295.21
T_{min}/K	295.15	296.65	303.15	301.37	248.15	284.95	295.21	293.87	295.21

Table 3 (Continued)

Ketones and Aldehydes (Continued)

	ethanal	propanal	butanal	2-methylpropanal	pentanal	3-methylbutanal	heptanal	octanal	benzaldehyde
T_{max}/K	295.15	296.65	333.15	301.37	374.15	362.35	295.21	293.87	295.21
P_{min}/MPa	13.89	13.89	35.61	13.89	5.00	5.00	13.89	13.89	13.89
P_{max}/MPa	138.00	138.00	276.58	138.00	50.08	50.08	138.00	138.00	138.00
RMSD/kg·m^{-3}	0.158	0.130	0.592	0.258	0.586	0.343	0.073	0.098	0.180
$RMSD_r$/%	0.019	0.016	0.069	0.031	0.075	0.044	0.009	0.012	0.017
bias/kg·m^{-3}	0.001	−0.002	−0.075	−0.033	0.005	−0.015	−0.007	0.005	0.032
N_p	10	10	25	10	24	16	10	10	10
±	−2	0	−5	0	−6	−4	−2	0	−2
s_w	0.989	1.021	1.140	1.028	1.092	0.963	0.924	1.016	1.035

Acids

	methanoic acid	ethanoic acid	propanoic acid	2-methyl-propanoic acid	octanoic acid	decanoic acid	dodecanoic acid	tetra-decanoic	hexa-decanoic acid
c_0	0.096327	0.092418	0.091314	0.087375	0.066987	0.093916	0.067638	0.173801	0.115340
b_0/MPa	148.7378	90.6714	98.6259	86.9541	66.0320	101.8285	75.0552	198.6292	136.1333
b_1/MPa·K^{-1}	−443.7460	−62.2302	−69.5680	−55.0296	−56.5565	−59.7045	−39.1829	−105.5458	−85.2892
b_2/MPa·K^{-2}		19.4216	20.6000		73.2502				
T_0/K	298.15	313.15	298.15	298.15	343.15	343.15	343.15	353.15	353.15
T_{min}/K	295.55	298.15	298.15	298.15	343.15	343.15	343.15	353.15	353.15
T_{max}/K	298.15	328.15	328.15	328.15	373.15	373.15	373.15	373.15	373.15
P_{min}/MPa	50.66	50.66	50.66	50.66	1.00	1.00	1.00	1.00	1.00
P_{max}/MPa	202.65	253.31	253.31	253.31	9.00	9.00	9.00	9.00	9.00
RMSD/kg·m^{-3}	0.047	0.098	0.091	0.272	0.068	0.059	0.054	0.054	0.043
$RMSD_r$/%	0.004	0.009	0.009	0.027	0.008	0.007	0.006	0.006	0.005
bias/kg·m^{-3}	0.002	0.000	0.003	0.004	0.006	−0.001	0.000	0.001	0.000
N_p	6	12	15	15	30	30	30	25	25
±	2	2	3	−1	4	0	−2	1	1
s_w	0.036	0.086	0.088	0.266	0.956	1.017	0.939	0.929	0.855

Esters

	methyl ethanoate	ethyl ethanoate	1-methylethyl ethanoate	1,2,3-propane-triyl tri-ethanoate	propyl propanoate	3-methylbutyl propanoate	methyl hexanoate	nonyl hexanoate	1,2,3-propane-triyl tri-hexanoate
c_0	0.087851	0.089409	0.106954	0.098843	0.103066	0.085373	0.091386	0.093890	0.095581
b_0/MPa	94.1389	91.8722	94.1343	145.0897	95.8443	89.9136	70.7425	85.5588	130.3507
b_1/MPa·K^{-1}	−74.2636	−81.9526	−103.4575	−53.7953	−71.1831	−67.6642	−44.7245	−48.2382	−59.5821
b_2/MPa·K^{-2}		49.0679	53.7186	31.4770	22.9642	16.2675	9.1129	12.2476	26.2163
b_3/MPa·K^{-3}		−18.2587						−1.6815	
T_0/K	273.15	273.15	297.17	368.15	300.00	298.15	294.99	289.00	323.15
T_{min}/K	253.15	253.15	297.17	273.15	300.00	298.15	294.99	289.00	273.15
T_{max}/K	313.15	343.15	367.20	368.15	400.00	423.15	408.85	530.72	368.15
P_{min}/MPa	19.66	5.00	5.00	49.03	5.00	5.00	4.90	4.90	49.03
P_{max}/MPa	156.75	156.75	49.10	1176.80	50.00	50.08	58.80	58.80	1176.80
RMSD/kg·m^{-3}	0.356	0.952	0.625	1.314	1.884	0.794	0.660	0.758	0.769
$RMSD_r$/%	0.035	0.106	0.071	0.102	0.215	0.102	0.078	0.094	0.070
bias/kg·m^{-3}	−0.003	−0.206	−0.088	0.084	0.118	−0.031	0.020	0.058	0.057
N_p	30	49	18	32	30	32	33	86	36
±	0	−1	0	0	−6	−2	−1	−2	0
s_w	1.020	1.018	0.999	1.016	0.960	0.908	1.044	0.939	0.990

	2-methyl-propyl 2-hydroxy-propanoate	pentyl 2-hydroxy-propanoate	methyl benzene-carboxylate	2-ethyl-hexyl benzene-carboxylate	methyl 2-hydroxy-benzene-carboxylate	pentyl 2-hydroxy-benzene-carboxylate	hexyl 2-hydroxy-benzene-carboxylate	methyl 2-methyl-2-propenoate
c_0	0.060907	0.034262	0.110587	0.097846	0.134172	0.165532	0.228551	0.094277
b_0/MPa	110.5039	42.2839	193.5738	157.7459	240.8968	204.0698	150.5257	98.2396
b_1/MPa·K^{-1}	−3.5979	−12.9463	−105.9694	−82.1159	−153.0592	−92.0613	−34.7764	−73.7312
b_2/MPa·K^{-2}			17.6617	14.0075	53.3590	23.1511	3.1064	8.3110
b_3/MPa·K^{-3}					−8.3332	−2.6619		
T_0/K	294.36	296.71	300.48	273.15	298.15	298.15	298.15	300.06
T_{min}/K	294.36	296.71	300.48	253.15	298.15	298.15	298.15	289.34
T_{max}/K	343.41	371.82	440.59	373.15	498.15	573.15	573.15	349.29
P_{min}/MPa	4.91	4.90	5.00	50.00	10.00	10.00	10.00	5.00
P_{max}/MPa	98.10	98.10	58.90	450.00	60.00	60.00	60.00	98.10
RMSD/kg·m^{-3}	0.554	0.920	0.466	0.543	0.372	0.484	0.213	0.430
$RMSD_r$/%	0.055	0.095	0.044	0.050	0.034	0.049	0.028	0.045
bias/kg·m^{-3}	0.079	0.089	−0.020	0.005	0.035	−0.019	−0.023	−0.008
N_p	29	37	49	59	54	71	72	61
±	5	−3	1	5	8	−1	−6	−9
s_w	1.193	0.949	0.999	0.897	0.957	1.099	0.934	0.978

Table 3 (Continued)

	Esters (Continued)							
	nonyl 2-methyl-2-propenoate	methyl (*Z*)-9-octadecenoate	diethyl 2,2-bis(phenylmethyl)propane-1,3-dioate	diethyl butane-1,4-dioate	dipropyl butane-1,4-dioate	dinonyl butane-1,4-dioate	dibutyl 1,2-dibenzenedicarboxylate	4-methyl-1,3-dioxolan-2-one
c_0	0.093482	0.096785	0.103806	0.057476	0.073591	0.495408	0.091695	0.092963
b_0/MPa	124.1357	107.1134	180.8024	81.6161	115.1185	376.2686	140.4724	181.5743
b_1/MPa·K^{-1}	−73.4228	−79.1092	−31.3735	−62.4077	−72.1588	−82.6642	−75.1749	
b_2/MPa·K^{-2}	13.7277	−27.3425				8.5461	−14.5783	
T_0/K	292.37	368.15	368.15	295.65	288.15	298.15	323.15	298.15
T_{min}/K	292.37	273.15	273.15	295.65	288.15	298.15	273.15	298.15
T_{max}/K	473.43	368.15	368.15	347.15	347.95	573.15	368.15	298.15
P_{min}/MPa	5.00	49.03	49.03	5.00	5.00	10.00	49.03	50.00
P_{max}/MPa	98.20	980.67	490.33	49.10	49.10	60.00	1176.80	200.00
RMSD/kg·m^{-3}	0.461	0.388	1.225	0.429	0.858	0.275	0.929	0.095
RMSD$_r$/%	0.055	0.041	0.106	0.042	0.085	0.031	0.080	0.008
bias/kg·m^{-3}	−0.019	−0.009	0.066	−0.025	0.083	−0.029	0.036	0.001
N_p	77	21	12	18	22	72	34	4
±	1	−5	2	−4	8	−6	2	−2
s_w	1.102	0.949	1.060	1.037	0.981	1.183	1.058	0.861

[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.

Table 6) are also significantly higher (0.5%) compared to other alkanones.

In the case of 2-octanone two available data sets are mutually inconsistent. A more precise data set by Apaev et al. [78-apa/ker] (lower RMSD and the experimental uncertainty about 0.1% in density declared by the authors) was, however, retained, taking into account that the values from Atoyan's laboratory were rejected for most of the other alkanones. The values of isothermal compressibility calculated from the fit are also reasonable, yielding an average deviation from literature values (see Table 5) of −5.7%, while those calculated from a tentative fit of data by Atoyan and Mamedov [75-ato/mam] showed an average deviation −8.5% with a maximum at 273.15 K (−14.1%).

The data sets available for cyclohexanone are in good mutual agreement. It is, however, worth mentioning that the values retained in the evaluation were not direct experimental ones (Table 2). The isothermal compressibility calculated from the fit differs from the value obtained from literature data (Table 5) by −6.6%.

Recently, Malhotra and Woolf [92-mal/woo] proposed generalized formulas for the parameters C and B of the Tait equation to calculate the volume ratio of liquid alkanones derived on the basis of their data for 2-propanone and 2-butanone [91-mal/woo, 92-mal/woo] in the reduced temperature range $0.54 \le T/T_c \le 0.62$. The formulas proved to be successful also for 3-pentanone [93-mal/pri]. In Table 6 the values of relative density, $\rho_{rel} = \rho(T,P)/\rho(T,P_{ref})$ calculated from the fits in Table 3 are compared with those calculated from the generalized relations of Malhotra and Woolf. The deviations $\{\rho_{rel}$(Table 3) $- \rho_{rel}$[92-mal/woo]$\}/\rho_{rel}$[92-mal/woo] observed for 2-propanone and 2-butanone are either within or close to the experimental error. Larger deviations for 2-butanone are found in the temperature range that exceeds the experimental range of Malhotra's data [92-mal/woo]. Since the generalized formulas were derived from data measured for the first two members only of the homologous series (2-propanone, 2-butanone) in a limited temperature range, the comparison presented in Table 6 for other alkanones is the comparison with the values obtained by an extensive extrapolation (in the sense of extrapolation beyond both the temperature range and particularly the range within the homologous series). Therefore, the significance of this comparison is, taking also into account the fact that one experimental data set only was available for some alkanones (see Table 2), rather low. However, the predictions using the Malhotra and Woolf generalized equations agree with the existing experimental data within about 0.5% (on average) and similar uncertainty might be expected for other members of the alkanone homologous series.

Aldehydes (Alkanals and Benzaldehyde). Data for members of the homologous series of aldehydes are very scarce. The analysis of literature data shows that values reported by Chaudhuri et al. [68-cha/sta] are likely to be systematically higher (by 10 kg·m^{-3} in density) since they show large positive deviations from both the repeated measurements performed in the extended temperature range in the same laboratory for butanal [71-run/sta] and the values for 3-methylbutanal reported by Mamedov et al. [75-mam/gus]. Therefore the data from [68-cha/sta] were not retained in the fits for these two alkanals. However, to provide an internally consistent set of the parameters of eq 1 for all data reported in the paper [68-cha/sta] the additional correlations, where only values from this source were retained, were performed yielding the following results.

Butanal: $c_0 = 0.099\,158$, $b_0 = 81.6468$ MPa, $T_{min} = T_{max} = 302.04$ K, $P_{max} = 138.00$ MPa, RMSD = 0.226 kg·m^{-3}, RMSD$_r$ = 0.027%, bias = 0.023 kg·m^{-3}, $N_p = 10$, ± = 2.

3-Methylbutanal: $c_0 = 0.077\,919$, $b_0 = 51.0029$ MPa, $T_{min} = T_{max} = 300.37$ K, $P_{max} = 138.00$ MPa, RMSD = 1.081 kg·m^{-3}, RMSD$_r$ = 0.131%, bias = 0.148 kg·m^{-3}, $N_p = 10$, ± = 2.

Carboxylic Acids. The situation is similar to that for aldehydes. Except for methanoic acid, one data set only was found for each carboxylic acid. Two sets for methanoic acid, generated using the reported parameters of the Tait equation ([63-and], [71-kor]), were correlated together. Low deviations of the fit (Table 3) and apparent agreement of the two sets (Table 4) are rather artificial, since values for two isotherms, close each other, were correlated. The large absolute value of the parameter b_1, which is, however, qualitatively correct being negative, indicates that the temperature dependence of density at elevated pressures might be incorrect and thus any extrapolation in temperature using the final fit is not advisable. The fits of data reported by Korpela [71-kor] for other acids (ethanoic, propanoic, 2-methylpropanoic) are recorrelations of the values generated using Tait parameters reported in the original paper for each temperature separately. The characteristic deviations of these fits (RMSD, RMSD$_r$, bias) should not be, therefore, regarded as criteria of the quality

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]
				3-Oxapentane (Diethyl Ether)						
13-bri					4.884	0.560	−4.411	85	−75	o
31-bri	303.15	348.15	49.1	1176.9	1.118	0.123	0.183	26	4	e
57-wal/ric								0	0	o
68-ski/cus					4.213	0.477	−3.223	11	−7	o
69-bra/fre	303.15	303.15	100.0	400.0	1.541	0.184	−1.144	7	−5	o
92-saf/mad					13.994	1.910	−9.168	22	−12	(o)
				4-Oxaheptane (Di-*n*-propyl Ether)						
68-ski/cus					8.482	1.072	−8.309	2	−2	o
92-saf/mad-1	294.30	374.50	4.9	98.1	1.361	0.183	0.224	40	6	o
				2,4-Dimethyl-3-oxapentane (Diisopropyl Ether)						
70-sch/eck	303.15	323.15	106.8	511.3	3.161	0.363	0.134	7	1	o
96-gov/let	288.15	328.15	0.5	8.0	0.179	0.025	0.051	45	3	o
				5-Oxanonane (Di-*n*-butyl Ether)						
94-sen	298.15	328.15	5.1	203.7	0.233	0.029	0.020	90	−2	o
				6-Oxaundecane (Di-*n*-pentyl Ether)						
49-bri	298.15	298.15	49.0	98.1	1.070	0.129	−0.284	2	0	o
92-saf/mad	296.64	456.82	4.9	98.1	1.437	0.190	0.051	78	6	o
				8-Oxapentadecane (Di-*n*-heptyl Ether)						
93-saf/oso	293.00	553.00	19.6	98.1	1.793	0.228	−0.095	113	−13	o
				3,3-Dimethyl-2-oxabutane (Methyl *tert*-Butyl Ether)						
94-sen	298.15	328.15	5.4	207.7	0.915	0.113	0.077	89	−11	o
96-gov/let	288.15	328.15	0.5	8.0	0.297	0.040	0.008	45	1	o
				4,4-Dimethyl-3-oxapentane (Ethyl *tert*-Butyl Ether)						
94-sen	298.15	328.15	5.6	207.2	0.483	0.062	0.015	90	0	o
				3,3-Dimethyl-2-oxapentane (Methyl *tert*-Pentyl Ether)						
94-sen	298.15	328.15	5.6	203.8	0.341	0.042	−0.040	90	−16	o
96-gov/let	288.15	328.15	0.5	8.0	0.140	0.018	0.046	45	23	o
				2,5-Dioxahexane (Ethylene Glycol Dimethyl Ether)						
78-sha/bai					1.859	0.216	−1.841	12	−12	e
94-sen	298.15	328.15	5.6	204.8	0.225	0.025	0.028	90	10	o
				2,5,8-Trioxanonane (Diethylene Glycol Dimethyl Ether)						
94-sen	298.15	328.15	5.1	202.8	0.173	0.018	0.013	90	8	o
				4,7,10-Trioxatridecane (Diethylene Glycol Dipropyl Ether)						
81-sha/abd	298.15	348.15	2.2	35.9	0.392	0.045	−0.114	22	−6	e
				2,5,8,11,14-Pentaoxapentadecane (Tetraethylene Glycol Dimethyl Ether)						
90-sve/sid	293.15	293.15	2.0	10.0	0.007	0.001	−0.001	5	−1	o
				4-Oxa-1,6-heptadiene (Diallyl Ether)						
92-saf/gus	291.70	365.00	4.9	98.1	1.680	0.230	0.140	38	6	o
				Methoxybenzene (Methyl Phenyl Ether)						
68-ski/cus					4.194	0.403	−3.711	3	−3	o
70-kus/tas	298.15	353.15	39.2	196.1	0.158	0.015	0.000	20	2	o
				Tetrahydrofuran (Oxolane)						
70-sch/eck	303.15	323.15	212.3	517.0	2.554	0.254	−0.202	7	−1	o
71-ham/smi					6.825	0.727	−6.825	1	−1	o
83-nak/miy	298.15	298.15	101.3	101.3	1.248	0.132	−1.248	1	−1	o
87-hol/goe	293.15	293.15	2.0	10.0	0.011	0.001	−0.002	5	−1	o
96-gov/let	288.15	328.15	0.5	8.0	0.108	0.012	0.025	45	19	o
				Tetrahydropyran (Oxane)						
96-gov/let	288.15	328.15	0.5	8.0	0.094	0.011	−0.009	45	−5	o
				1,4-Dioxane						
66-kor/kos								0	0	o
68-pea/str	298.15	298.15	25.0	50.0	1.241	0.118	0.338	2	0	o
96-gov/let	288.15	328.15	0.5	8.0	0.097	0.009	0.010	45	3	o
				Furan						
78-fig/szw	209.00	257.00	11.0	897.0	2.385	0.213	0.001	185	49	o
				Dibenzofuran						
84-nas/siv	391.55	563.15	0.5	25.5	1.080	0.103	0.037	38	−2	o
				2-Propanone (Dimethyl Ketone)						
13-bri					7.784	0.880	−7.528	28	−28	o
51-new/wea					1.569	0.183	−1.569	1	−1	o
56-stu					6.248	0.738	−6.248	1	−1	o
57-wal/ric								0	0	o
66-win/pow[b]								0	0	o
67-ada/lai					2.558	0.305	−2.471	7	−7	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]
2-Propanone (Dimethyl Ketone)										
76-ato/mam					7.201	0.837	−3.856	16	−14	(o)
77-gup/han					2.203	0.283	2.188	8	8	e
80-rae/fin					15.986	1.799	−13.019	17	−17	e
87-hol/goe-1	293.15	293.15	2.0	10.0	0.160	0.020	0.142	5	5	o
87-nhu/bha	293.15	293.15	2.0	10.0	0.115	0.014	0.100	5	5	o
91-mal/woo	278.15	323.15	2.5	392.3	0.267	0.031	0.083	105	25	o
91-pap/zia	298.15	298.15	2.0	33.8	0.349	0.043	−0.309	9	−9	o
92-ego/gru					1.295	0.157	−1.054	5	−5	o
2-Butanone (Methyl Ethyl Ketone)										
63-and					2.848	0.313	−2.820	6	−6	o
74-ato/mam					12.678	1.649	8.745	243	67	(o)
76-ato/bag	373.15	473.15	60.8	162.1	2.533	0.324	−0.177	28	−4	(o)
77-lam/hun					3.288	0.391	−2.028	15	−5	o
92-mal/woo	278.15	338.15	2.3	282.5	0.300	0.034	0.040	137	7	o
2-Pentanone (Methyl *n*-Propyl Ketone)										
77-apa/ker	273.00	315.66	5.0	78.6	0.279	0.033	−0.054	18	−2	o
3-Pentanone (Diethyl Ketone)										
82-ato/mam					6.740	0.781	−5.871	27	−27	o
93-mal/pri	278.15	338.15	2.5	389.8	0.307	0.036	0.087	128	36	o
2-Hexanone (Methyl *n*-Butyl Ketone)										
79-ato	293.15	393.15	9.8	156.9	0.990	0.125	−0.132	53	3	o
4-Methyl-2-pentanone (Methyl Isobutyl Ketone)										
63-and	295.55	295.55	245.2	484.8	0.802	0.085	0.029	13	−3	o
4-Heptanone (Di-*n*-propyl Ketone)										
91-ato	273.00	403.00	10.0	160.0	1.102	0.129	−0.012	71	17	o
2-Octanone (Methyl *n*-Hexyl Ketone)										
75-ato/mam					2.207	0.263	−1.004	18	−14	(o)
78-apa/ker	273.15	374.31	5.0	78.6	0.550	0.067	−0.070	25	−7	(o)
Cyclopentanone										
69-bra/fre	298.15	298.15	50.0	400.0	5.847	0.565	−0.318	8	0	o
Cyclohexanone										
63-and	296.45	296.45	158.7	266.1	0.261	0.025	−0.231	3	−3	o
82-wis/wue	253.20	303.40	10.0	220.0	0.709	0.072	−0.027	93	11	o
Ethanal (Acetaldehyde)										
68-cha/sta	295.15	295.15	13.9	138.0	0.158	0.019	0.001	10	−2	o
Propanal (Propionaldehyde)										
68-cha/sta	296.65	296.65	13.9	138.0	0.130	0.016	−0.002	10	0	o
Butanal (Butyraldehyde)										
68-cha/sta								0	0	o
71-run/sta	303.15	333.15	35.6	276.6	0.592	0.069	−0.075	25	−5	o
2-Methylpropanal (Isobutyraldehyde)										
68-cha/sta	301.37	301.37	13.9	138.0	0.258	0.031	−0.033	10	0	o
Pentanal (Valeraldehyde)										
75-mam/gus	248.15	374.15	5.0	50.1	0.586	0.075	0.005	24	−6	o
3-Methylbutanal (Isovaleraldehyde)										
68-cha/sta					6.168	0.754	6.162	3	3	o
75-mam/gus	284.95	362.35	5.0	50.1	0.343	0.044	−0.015	16	−4	o
Heptanal (Enanthaldehyde)										
68-cha/sta	295.21	295.21	13.9	138.0	0.073	0.009	−0.007	10	−2	o
Octanal (Caprylic Aldehyde)										
68-cha/sta	293.87	293.87	13.9	138.0	0.098	0.012	0.005	10	0	o
Benzaldehyde										
68-cha/sta	295.21	295.21	13.9	138.0	0.180	0.017	0.032	10	−2	o
Methanoic Acid (Formic Acid)										
63-and	295.55	295.55	76.5	107.5	0.070	0.006	0.008	2	0	o
71-kor	298.15	298.15	50.7	202.7	0.028	0.002	−0.001	4	2	o
Ethanoic Acid (Acetic Acid)										
71-kor	298.15	328.15	50.7	253.3	0.098	0.009	0.000	12	2	o
Propanoic Acid (Propionic Acid)										
71-kor	298.15	328.15	50.7	253.3	0.091	0.009	0.003	15	3	o
2-Methylpropanoic Acid (Isobutyric Acid)										
71-kor	298.15	328.15	50.7	253.3	0.272	0.027	0.004	15	−1	o
Octanoic Acid (Caprylic Acid)										
92-ban/gar	343.15	373.15	1.0	9.0	0.068	0.008	0.006	30	4	o
Decanoic Acid (Capric Acid)										
92-ban/gar	343.15	373.15	1.0	9.0	0.059	0.007	−0.001	30	0	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]
				Dodecanoic Acid (Lauric Acid)						
92-ban/gar	343.15	373.15	1.0	9.0	0.054	0.006	0.000	30	−2	o
				Tetradecanoic Acid (Myristic Acid)						
92-ban/gar	353.15	373.15	1.0	9.0	0.054	0.006	0.001	25	1	o
				Hexadecanoic Acid (Palmitic Acid)						
92-ban/gar	353.15	373.15	1.0	9.0	0.043	0.005	0.000	25	1	o
				Methyl Ethanoate (Methyl Acetate)						
78-kum/iwa	253.15	313.15	19.7	156.8	0.356	0.035	−0.003	30	0	o
				Ethyl Ethanoate (Ethyl Acetate)						
49-bri					1.540	0.157	−1.402	3	−3	o
63-and								0	0	o
70-sch/eck					7.710	0.832	−7.150	4	−4	o
75-gus/kad	300.06	343.15	5.0	49.1	1.480	0.167	−0.781	17	−5	o
79-kum/iwa	253.15	313.15	19.7	156.8	0.473	0.050	0.100	32	4	o
				1-Methylethyl Ethanoate (Isopropyl Acetate)						
75-gus/kad	297.17	367.20	5.0	49.1	0.625	0.071	−0.088	18	0	o
				1,2,3-Propanetriyl Triethanoate (Glyceryl Triacetate; Triacetin)						
32-bri	273.15	368.15	49.0	1176.8	1.314	0.102	0.084	32	0	o[c]
				Propyl Propanoate (*n*-Propyl Propionate)						
78-gus/kli	300.00	400.00	5.0	50.0	1.884	0.215	0.118	30	−6	o
				3-Methylbutyl Propanoate (Isopentyl Propionate)						
76-gus/kli	298.15	423.15	5.0	50.1	0.794	0.102	−0.031	32	−2	o
				Methyl Hexanoate (Methyl Caproate)						
92-mus/gus	294.99	408.85	4.9	58.8	0.660	0.078	0.020	33	−1	o
				Nonyl Hexanoate (*n*-Nonyl Caproate)						
92-mus/gus-1	289.00	530.72	4.9	58.8	0.758	0.094	0.058	86	−2	o
				1,2,3-Propanetriyl Trihexanoate (Glyceryl Trihexanoate; Tricaproin)						
32-bri	273.15	368.15	49.0	1176.8	0.769	0.070	0.057	36	0	o[c]
				2-Methylpropyl 2-Hydroxypropanoate (Isobutyl Lactate)						
91-gus/kul	294.36	343.41	4.9	98.1	0.554	0.055	0.079	29	5	o
				Pentyl 2-Hydroxypropanoate (*n*-Pentyl Lactate)						
91-gus/kul-1	296.71	371.82	4.9	98.1	0.920	0.095	0.089	37	−3	o
				Methyl Benzenecarboxylate (Methyl Benzoate)						
94-mus/tag	300.48	440.59	5.0	58.9	0.466	0.044	−0.020	49	1	o
				2-Ethylhexyl Benzenecarboxylate (2-Ethylhexyl Benzoate)						
88-wal/lam	253.15	373.15	50.0	450.0	0.543	0.050	0.005	59	5	o
				Methyl 2-Hydroxybenzenecarboxylate (Methyl Salicylate)						
90-mus/gan-1	298.15	498.15	10.0	60.0	0.372	0.034	0.035	54	8	o
				Pentyl 2-Hydroxybenzenecarboxylate (*n*-Pentyl Salicylate)						
90-mus/gan-1	298.15	573.15	10.0	60.0	0.484	0.049	−0.019	71	−1	o
				Hexyl 2-Hydroxybenzenecarboxylate (*n*-Hexyl Salicylate)						
90-mus/gan-1	298.15	573.15	10.0	60.0	0.213	0.028	−0.023	72	−6	o
				Methyl 2-Methyl-2-propenoate (Methyl Methacrylate)						
87-gus/bai	289.34	349.29	5.0	98.1	0.430	0.045	−0.008	61	−9	o
				Nonyl 2-Methyl-2-propenoate (*n*-Nonyl Methacrylate)						
89-gus/bai	292.37	473.43	5.0	98.2	0.461	0.055	−0.019	77	1	o
				Methyl (*Z*)-9-Octadecenoate (Methyl Oleate)						
32-bri	273.15	368.15	49.0	980.7	0.388	0.041	−0.009	21	−5	o[c]
				Diethyl 2,2-Bis(phenylmethyl)propane-1,3-dioate (Diethyl Dibenzylmalonate)						
32-bri	273.15	368.15	49.0	490.3	1.225	0.106	0.066	12	2	o[c]
				Diethyl Butane-1,4-dioate (Diethyl Succinate)						
90-mus/gan-3	295.65	347.15	5.0	49.1	0.429	0.042	−0.025	18	−4	o
				Dipropyl Butane-1,4-dioate (Di-*n*-propyl Succinate)						
90-mus/gan-2	288.15	347.95	5.0	49.1	0.858	0.085	0.083	22	8	o
				Dinonyl Butane-1,4-dioate (Di-*n*-nonyl Succinate)						
91-mus/gan	298.15	573.15	10.0	60.0	0.275	0.031	−0.029	72	−6	o
				Dibutyl Benzene-1,2-dicarboxylate (Di-*n*-butyl Phthalate)						
32-bri	273.15	368.15	49.0	1176.8	0.929	0.080	0.036	34	2	o[c]
				4-Methyl-1,3-dioxolan-2-one (Propylene Carbonate)						
92-uos/kit	298.15	298.15	50.0	200.0	0.095	0.008	0.001	4	−2	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] All three sets (see Table 2). [c] 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. 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
		3-Oxapentane		
303.15	2.03 ± 0.03	2.110	−3.8	[72-dri/wil],[c] [83-hal/gun][d]
		2.082	−2.5	[82-bro/lop][e]
308.15	2.13 ± 0.03	2.269	−6.1	[72-dri/wil],[c] [83-hal/gun][d]
		4-Oxaheptane		
298.15	1.76 ± 0.07	1.484	18.6	[72-dri/wil],[c] [85-oba/ood][d]
		1.442	22.1	[83-kim/tre],[f] [92-saf/mad-1],[g] [96-zab/ruz][h]
		5-Oxanonane		
298.15	1.209 ± 0.004	1.223	−1.1	[72-dri/wil],[c] [85-oba/ood][d]
		6-Oxaundecane		
298.15	0.93 ± 0.02	1.080	−13.9	[72-dri/wil],[c] [85-oba/ood][d]
		4,4-Dimethyl-3-oxapentane		
298.15	1.782 ±0.012	1.771	0.9	[95-mie/osw][e]
313.15	2.083 ± 0.015	1.990	4.7	[95-mie/osw][e]
		2,5,8-Trioxanonane		
298.15	0.817 ± 0.002	0.823	−0.7	[82-tre/hal],[f] [94-sen],[g] [96-zab/ruz][h]
		0.814	0.3	[93-ami/pha],[f] [94-sen],[g] [96-zab/ruz][h]
303.15	0.848 ± 0.002	0.853	−0.6	[93-ami/pha],[f] [94-sen],[g] [96-zab/ruz][h]
308.15	0.881 ± 0.002	0.877	0.4	[93-ami/pha],[f] [94-sen],[g] [96-zab/ruz][h]
313.15	0.916 ± 0.002	0.911	0.5	[93-ami/pha],[f] [94-sen],[g] [96-zab/ruz][h]
		Tetrahydrofuran		
293.15	0.957 ± 0.002	0.933	2.6	[71-des/bha],[f] *i*, [96-zab/ruz][h]
298.15	1.010 ± 0.006	0.992	1.8	[89-ram/kud],[f] *i*, [96-zab/ruz][h]
		0.859	17.6	[89-ram/kud],[f] [96-gov/let],[g,j] [96-zab/ruz][h]
		0.979	3.2	[79-kiy/dar],[f] *i*, [96-zab/ruz][h]
		0.846	19.4	[79-kiy/dar],[f] [96-gov/let],[g,j] [96-zab/ruz][h]
303.15	1.06 ± 0.01	1.016	4.3	[49-wei],[f] *i*, [96-zab/ruz][h]
308.15	1.12 ± 0.02	1.057	6.0	[71-des/bha],[f], *i*, [96-zab/ruz][h]
		Tetrahydropyran		
298.15	0.99 ± 0.02	0.994	−0.4	[91-spa/lep][e]
		1,4-Dioxane		
293.15	0.75 ± 0.02	0.701	7.0	[44-sch],[f] [92-sak],[g] [96-zab/ruz][h]
		0.601	24.8	[44-sch],[f] [96-gov/let],[g,k] [96-zab/ruz][h]
298.15	0.79 ± 0.02	0.738	7.0	[71-des/bha][e]
		0.744	6.2	[90-aic/cos],[f] [92-sak],[g] [96-zab/ruz][h]
		0.627	26.0	[90-aic/cos],[f] [96-gov/let],[g,j] [96-zab/ruz][h]
		0.637	24.0	[90-aic/cos],[f] [96-gov/let],[g,k] [96-zab/ruz][h]
303.15	0.82 ± 0.02	0.768	6.8	[49-wei],[f] [92-sak],[g] [96-zab/ruz][h]
		0.650	26.2	[49-wei],[f] [96-gov/let],[g,k] [96-zab/ruz][h]
308.15	0.86 ± 0.03	0.797	7.9	[71-des/bha],[f] [92-sak],[g] [96-zab/ruz][h]
		0.669	28.6	[71-des/bha],[f] [96-gov/let],[g,k] [96-zab/ruz][h]
		2-Propanone		
293.15	1.234 ± 0.004	1.269	−2.8	[78-ric][e]
		1.271	−2.9	[71-ric/rog][e]
298.15	1.293 ± 0.004	1.324	−2.3	[78-ric][e]
		1.286	0.5	[71-des/bha][e]
308.15	1.419 ± 0.004	1.398	1.5	[71-des/bha][e]
313.15	1.485 ± 0.004	1.561	−4.9	[29-fre/hub][e]
		1.536	−3.3	[71-ric/rog][e]
318.15	1.553 ± 0.004	1.523	2.0	[71-des/bha][e]
323.15	1.623 ± 0.005	1.657	−2.0	[29-fre/hub],[f] [91-trc],[g] [96-zab/ruz][h]
		2-Butanone		
283.15	1.032 ± 0.002	1.022	1.0	[49-lag/mcm],[f] [91-trc],[g] [96-zab/ruz][h]
293.15	1.120 ± 0.002	1.116	0.4	[78-ric][e]
		1.117	0.3	[76-ato/bag],[f] [91-trc],[g] [96-zab/ruz][h]
298.15	1.167 ± 0.002	1.188	−1.8	[78-ric][e]
303.15	1.216 ± 0.003	1.214	0.2	[78-red/nai],[f] [91-trc],[g] [96-zab/ruz][h]
313.15	1.322 ± 0.003	1.328	−0.5	[76-ato/bag],[f] [91-trc],[g] [96-zab/ruz][h]
333.15	1.566 ± 0.005	1.593	−1.6	[76-ato/bag],[f] [91-trc],[g] [96-zab/ruz][h]
353.15	1.87 ± 0.01	1.940	−3.6	[76-ato/bag],[f] [91-trc],[g] [96-zab/ruz][h]
		2-Pentanone		
293.15	0.97 ± 0.02	1.051	−7.7	[78-ric][e]
298.15	1.02 ± 0.02	1.092	−6.6	[78-ric][e]
303.15	1.07 ± 0.02	1.141	−6.2	[78-sre/nai],[f] [91-trc],[g] [96-zab/ruz][h]
313.15	1.20 ± 0.02	1.234	−2.7	[78-sre/nai],[f] [91-trc],[g] [96-zab/ruz][h]
		3-Pentanone		
293.00	1.002 ± 0.003	1.018	−1.6	[82-ato/mam],[f] [93-mal/pri],[g] [96-zab/ruz][h]
303.15	1.083 ± 0.004	1.114	−2.7	[76-red/nai],[f] [93-mal/pri],[g] [96-zab/ruz][h]
313.00	1.169 ± 0.004	1.190	−1.8	[82-ato/mam],[f] [93-mal/pri],[g] [96-zab/ruz][h]
313.15	1.171 ± 0.004	1.209	−3.1	[76-red/nai],[f] [93-mal/pri],[g] [96-zab/ruz][h]
333.00	1.373 ± 0.006	1.405	−2.3	[82-ato/mam],[f] [93-mal/pri],[g] [96-zab/ruz][h]

Table 5 (Continued)

	β_T/GPa^{-1}			
T/K	eq 1[a]	lit.	$\delta\beta_T$/%[b]	ref
		2-Hexanone		
293.15	0.80 ± 0.02	0.995	−19.8	[78-ric][e]
		0.973	−17.8	[79-ato],[f] [91-trc],[g] [96-zab/ruz][h]
298.15	0.84 ± 0.02	1.014	−17.3	[78-ric][e]
313.15	0.97 ± 0.02	1.131	−14.2	[79-ato],[f] [91-trc],[g] [96-zab/ruz][h]
333.15	1.17 ± 0.03	1.326	−11.8	[79-ato],[f] [91-trc],[g] [96-zab/ruz][h]
353.15	1.40 ± 0.03	1.570	−10.8	[79-ato],[f] [91-trc],[g] [96-zab/ruz][h]
373.15	1.66 ± 0.04	1.882	−11.8	[79-ato],[f] [91-trc],[g] [96-zab/ruz][h]
		4-Heptanone		
303.00	0.87 ± 0.02	1.020	−14.7	[91-ato],[f,g] [96-zab/ruz][h]
323.00	1.04 ± 0.02	1.177	−11.6	[91-ato],[f,g] [96-zab/ruz][h]
343.00	1.24 ± 0.03	1.366	−9.2	[91-ato],[f,g] [96-zab/ruz][h]
		2-Octanone		
273.15	0.73 ± 0.02	0.797	−8.4	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
293.15	0.84 ± 0.02	0.885	−5.2	[78-ric][e]
		0.914	−8.1	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
298.15	0.87 ± 0.02	0.899	−3.2	[78-ric][e]
313.15	0.97 ± 0.02	1.053	−7.9	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
333.15	1.14 ± 0.03	1.219	−6.5	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
353.15	1.36 ± 0.04	1.421	−4.3	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
373.15	1.64 ± 0.06	1.673	−2.0	[75-ato/mam],[f] [91-trc],[g] [96-zab/ruz][h]
		Cyclohexanone		
303.15	0.67 ± 0.01	0.717	−6.6	[76-rao/nai],[f] [82-wis/wue],[g] [96-zab/ruz][h]
		Benzaldehyde		
295.21	0.61 ± 0.01	0.573	6.5	*l*
		Methanoic Acid		
295.55	0.601 ± 0.001	0.617	−2.6	[64-lut/sol][e]
		0.613	−2.0	[83-goo/whi],[f] [84-trc],[g] [96-zab/ruz][h]
298.15	0.647 ± 0.002	0.627	3.2	[64-lut/sol][e]
		0.620	4.4	[83-goo/whi],[f] [84-trc],[g] [96-zab/ruz][h]
		Ethanoic Acid		
298.15	0.919 ± 0.003	0.954	−3.7	[64-lut/sol][e]
		0.918	0.1	[65-for/moo],[f] [83-hal/gun],[g] [96-zab/ruz][h]
313.15	1.018 ± 0.003	1.045	−2.6	[64-lut/sol][e]
		1.003	1.5	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
323.15	1.091 ± 0.004	1.112	−1.9	[71-ric/rog][e]
		1.118	−2.4	[64-lut/sol][e]
		1.069	2.1	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
328.15	1.129 ± 0.004	1.158	−2.5	[64-lut/sol][e]
		1.072	5.3	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
		Propanoic Acid		
298.15	0.925 ± 0.002	0.939	−1.5	[64-lut/sol][e]
		0.930	−0.5	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
313.15	1.029 ± 0.003	1.043	−1.3	[64-lut/sol][e]
		1.022	0.7	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
328.15	1.146 ± 0.004	1.164	−1.5	[64-lut/sol][e]
		1.124	2.0	[83-goo/whi],[f] [83-hal/gun],[g] [96-zab/ruz][h]
		Methyl Ethanoate		
298.15	1.16 ± 0.01	1.158	0.2	[93-ami/pha],[f] [78-kum/iwa],[g] [96-zab/ruz][h]
299.15	1.17 ± 0.01	1.174	−0.4	[53-par/bak],[f] [78-kum/iwa],[g] [96-zab/ruz][h]
303.15	1.22 ± 0.01	1.212	0.6	[93-ami/pha],[f] [78-kum/iwa],[g] [96-zab/ruz][h]
308.15	1.29 ± 0.02	1.273	1.3	[93-ami/pha],[f] [78-kum/iwa],[g] [96-zab/ruz][h]
313.15	1.36 ± 0.02	1.337	1.7	[93-ami/pha],[f] [78-kum/iwa],[g] [96-zab/ruz][h]
		Ethyl Ethanoate		
273.15	0.97 ± 0.01	0.980	−1.0	[71-ric/rog][e]
293.15	1.16 ± 0.02	1.133	2.4	[71-ric/rog][e]
298.15	1.20 ± 0.02	1.206	−0.5	[93-ami/rai],[f] [69-trc],[g] [96-zab/ruz][h]
323.15	1.47 ± 0.02	1.480	−0.7	[71-ric/rog][e]
		Methyl Benzenecarboxylate		
298.15	0.56 ± 0.01[m]	0.618	−9.4	[93-ami/rai],[f] [91-gar/mir],[g] [96-zab/ruz][h]
		4-Methyl-1,3-dioxolan-2-one		
298.15	0.512 ± 0.003	0.518	−1.2	[86-bot/bre][e,n]
		0.480	6.6	[86-bot/bre][e,o]

[a] Uncertainty is estimated as ±2s, where s is a standard deviation derived from a covariance matrix of each fit. [b] $[\beta_T(\text{eq 1}) - \beta_T(\text{lit.})]100/\beta_T(\text{lit.})$. [c] Thermal pressure coefficient, $\gamma_V = (\partial P/\partial T)_V$. [d] Thermal expansivity, $\alpha_P = (1/V)(\partial V/\partial T)_P$. [e] Isothermal compressibility, $\beta_T = -(1/V)(\partial V/\partial P)_T$. [f] Speed of sound. [g] Density and thermal expansivity. [h] Isobaric heat capacity. [i] Density and thermal expansivity were obtained from smoothed density data from 83-ing/gro, 87-hol/goe, and 89-ram/kud. [j] α_P taken from the text in 96-gov/let. [k] α_P calculated from the smoothing equation presented in Appendix II. [l] Literature value was obtained by linear interpolation between $\beta_T(T = 293.15\ \text{K}) = 0.566\ \text{GPa}^{-1}$ and $\beta_T(T = 299.75\ \text{K}) = 0.587\ \text{GPa}^{-1}$ evaluated from speeds of sound from 44-sch and 53-par/bak, smoothed densities from 75-amb/con, and heat capacities from 96-zab/ruz. [m] Extrapolated. [n] Evaluated from piezometric measurements. [o] Evaluated from densitometric measurements.

Table 6. Comparison of Relative Densities, $\rho_{rel} = \rho(T,P)/\rho(T,P_{ref})$, (See Eq 1), of Alkanones Calculated from the Fits in Table 3 with the Generalized Tait Equation of Malhotra and Woolf [92-mal/woo]

alkanone	T range[a]/K	T_r range[b]	P_{max}[a]/MPa	$RMSD_r$/%	$bias_r$[c]/%	max. dev[c]/%
2-propanone	278−323	0.55−0.64	309	0.070	−0.012	−0.177
2-butanone	278−353	0.52−0.66	280	0.074	0.019	−0.225
2-pentanone	273−313	0.49−0.56	78	0.156	−0.108	−0.362
3-pentanone	278−338	0.50−0.60	390	0.165	−0.124	−0.305
2-hexanone	293−393	0.50−0.67	160	0.531	−0.444	−1.195
4-methyl-2-pentanone	296	0.51	480	0.308	0.297	0.388
4-heptanone	273−403	0.45−0.67	160	0.384	0.163	0.840
2-octanone	273−373	0.43−0.59	80	0.615	0.490	1.715

[a] The temperature and pressure ranges are up to T_{max} (Table 3) or normal boiling temperature, whichever is lower, and P_{max} (Table 3), respectively. The relative density values used in a comparison were generated in 5 K and $P_{max}/10$ increments. [b] Critical temperatures were taken from 95-pul/gud; that of 4-methyl-2-pentanone (575.5 ± 0.5 K) was from 93-cda. [c] $\{\rho_{rel}$(Table 3) − ρ_{rel}[92-mal/woo]$\}100/\rho_{rel}$[92-mal/woo].

Table A1. Parameters, a_i, of Functions A1 and A2 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, ±, References to the Density Data, ref(ρ), and References to Saturated Vapor Pressure Data, ref(P_{ref})

	3-oxapentane	2,5-dioxahexane	4,7,10-trioxatridecane	2-propanone	2-butanone	2-octanone
eq	A1	A1	A2	A1	A1	A1
a_0	1.877396	−1.951904	1123.8823	1.838053	2.132989	5.598593
a_1	0.220896	9.590776	−69.3648	0.582830	0.934622	−12.662290
a_2	0.621815	−5.635101	−3.15008	−0.100291	−1.953535	15.459716
a_3				0.570410	1.940789	−5.297409
ρ_c/kg·m^{-3} [a]	264.724	332.554		277.895	270.064	258.000
T_c/K	466.74	536.00		508.10	536.78	632.70
T_{min}/K	293.15	288.00	298.15	178.50	193.15	273.15
T_{max}/K	370.00	333.00	348.15	508.10	536.78	433.15
RMSD/kg·m^{-3}	0.035	0.605	0.112	0.107	0.135	0.024
$RMSD_r$/%	0.005	0.070	0.013	0.025	0.026	0.003
bias/kg·m^{-3}	0.000	0.000	0.000	0.000	−0.005	0.001
N_p	8	9	7	35	36	18
±	0	−1	−1	1	2	−4
ref(ρ)	83-hal/gun	78-sha/bai	81-sha/abd	91-trc	91−trc	91−trc
ref(P_{ref})	83-mcg				83−mcg	

[a] Given with three decimal points since critical densities were calculated from rounded values of critical molar volumes recorded in the database.

of data. Low scatter of the generated $P-\rho-T$ values used in correlations results also in low values of standard deviations of values of isothermal compressibility calculated from the fits. The agreement with the values from the literature is quite satisfactory (the deviations below 6% for ethanoic acid and below 2% for propanoic acid; see Table 5).

Esters. One experimental data set only was available for all but one ester. In the case of ethyl ethanoate two data sets ([79-kum/iwa], [75-gus/kad]) are in acceptable agreement at lower temperatures; the values reported by Guseinov and Kadzarov [75-gus/kad] for higher temperatures (where no original reference densities were available) are not, however, consistent with smoothed saturated-liquid densities from 69-trc, and thus the temperature range of the fit was limited up to 343 K to avoid an inflection point on the $B(T)$ curve. The agreement of calculated values of isothermal compressibility at atmospheric pressure with data from the literature is satisfactory (see Table 5). An obvious typographical error was found in the data table presented for propyl propanoate by Guseinov and Klimova [78-gus/kli]; the value of $\rho(T =$ 300 K, $P = 0.1$ MPa) should be 873.8 kg·m^{-3}. With this value of the reference density all values along the isotherm 300 K become consistent with other reported data. Similarly, the reference density $\rho(T = 311.48$ K, $P = 0.1$ MPa) = 932.4 kg·m^{-3} reported for methyl 2-methyl-2-propenoate by Guseinov et al. [87-gus/bai] is erroneous; the correct value 923.4 kg·m^{-3}, deduced from a comparison with the smoothed value at atmospheric pressure (see Table A2 in Appendix II), was used in the correlations. Values at lower pressures (up to 10 MPa) for 3-methylbutyl propanoate [76-gus/kli], 2-methylpropyl 2-hydroxypropanoate [91-gus/kul], and pentyl 2-hydroxypropanoate [91-gus/kul-1] were mostly rejected due to large deviations compared to other isobars. Unusually high uncertainty (±5%) is declared by the authors [88-wal/lam] for measurements of density of 2-ethylhexyl benzenecarboxylate; fitting their data showed, however, low scatter and good consistency, contrary to the declared accuracy of measurements. The value reported by Mustafaev et al. [90-mus/gan-1] for pentyl 2-hydroxybenzenecarboxylate at $T = 298.15$ K and $P = 60$ MPa was rejected, being obviously erroneous (typographical error, correct value should be probably 1086.1 kg·m^{-3}). With the original value it was impossible to find reasonable values of adjustable parameters $\bar{c}$ and $\bar{b}$ for the entire data set. Data measured for 4-methyl-1,3-dioxolan-2-one (propylene carbonate) were correlated by 92-uos/kit using the Tait equation; our parameters c_0 and b_0 differ slightly from their values since the weighted least squares fit using experimental uncertainties declared by Uosaki and Kitaura was performed.

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Table A2. Parameters a_i of Smoothing Functions A1 or A2 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
					4-Oxaheptane					
A1	5.58970	−9.79084	7.29440		261.991	530.60	294.30	374.50	0.173	92-saf/mad-1
					2,4-Dimethyl-3-oxapentane					
A2	1072.556	−153.742	11.667				288.15	328.15	0.035	96-gov/let
					5-Oxanonane					
A1	3.86694	−5.02658	4.11614		260.461	580.00	293.15	328.15	0.039	94-sen
					6-Oxaundecane					
A2	1057.381	−96.713	1.388				296.64	456.82	1.085	92-saf/mad
					8-Oxapentadecane					
A2	1045.472	−83.989	−0.061				293.00	553.00	0.252	93-saf/oso
					3,3-Dimethyl-2-oxabutane					
A1	5.11100	−9.01518	6.95032		277.200	497.10	293.15	328.15	0.111	94-sen
					4,4-Dimethyl-3-oxapentane					
A2	1099.724	−137.703	5.184				293.15	328.15	0.165	94-sen
					3,3-Dimethyl-2-oxapentane					
A2	1025.918	−78.203	−2.932				293.15	328.15	0.035	94-sen
					2,5-Dioxahexane					
A1	2.38730	−2.12662	2.26726		332.554	536.00	293.15	328.15	0.049	94-sen
					2,5,8-Trioxanonane					
A1	3.12088	−3.47744	3.22672		318.706	625.30	293.15	328.15	0.031	94-sen
					2,5,8,11,14-Pentaoxapentadecane					
A2	1011.110						293.15	293.15		90-sve/sid
					4-Oxa-1,6-heptadiene					
A2	1008.412	−104.677	2.626				291.70	365.00	0.842	92-saf/gus
					Methoxybenzene					
A1	0.28525	3.87691	−1.58385		335.839	645.60	298.15	353.15	0.071	70-kus/tas
					Tetrahydrofuran					
A1	2.83393	−2.57687	2.41398		321.906	540.10	278.15	318.15	0.185	*b*, *i*
					Tetrahydropyran					
A1	10.04322	−20.40679	13.18624		327.505	572.20	288.15	328.15	0.327	96-gov/let
					1,4-Dioxane					
A1	9.28035	−17.86459	11.34313		370.195	587.00	288.15	328.15	0.300	96-gov/let
					Furan					
A2	1464.660	−294.417	42.262				209.00	257.00	1.414	78-fig/szw[c]
					Dibenzofuran					
A2	1720.181	−259.830	32.168	−1.953			391.55	563.15	0.009	84-nas/siv
					2-Pentanone					
A1	2.69374	−2.45770	2.54994		286.159	561.08	233.15	373.15	0.059	91-trc[d,i]
					3-Pentanone					
A1	4.17653	−4.95315	4.06914		256.000	560.60	278.15	338.15	0.003	93-mal/pri
					2-Hexanone					
A1	4.13574	−5.57604	4.59059		267.095	587.00	293.15	393.15	0.019	79-ato
					4-Heptanone					
A2	1080.148	−88.701	−0.353				273.00	403.00	0.648	91-ato
					Cyclopentanone					
A2	943.000						298.15	298.15		69-bra/fre
					Cyclohexanone					
A1	0.87043	2.31845	−0.47564		314.567	653.00	253.20	303.40	0.135	82-wis/wue
					Butanal					
A1	2.58929	0.22314			259.378	524.00	303.15	333.15	0.290	71-run/sta
					Pentanal					
A2	560.204	224.899	−48.533				248.15	374.15	1.714	75-mam/gus
					3-Methylbutanal					
A2	913.687	11.1330	−17.428				284.95	362.35	0.000[e]	75-mam/gus
					Methanoic Acid					
A2	1213.6						298.15	298.15		71-kor
					Ethanoic Acid					
A1	0.50162	7.48628	−11.10569	6.09003	351.185	592.71	293.15	490.00	0.063	83-hal/gun[f,i]
					Propanoic Acid					
A1	−1.08282	13.12210	−18.34957	9.33221	333.691	612.00	288.15	490.00	0.040	83-hal/gun[g,i]
					2-Methylpropanoic Acid					
A2	1245.170	−101.337					298.15	328.15	0.047	71-kor

Table A2 (Continued)

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
					Octanoic Acid					
A2	1120.486	−67.062	−1.762				343.15	373.15	0.060	92-ban/gar
					Decanoic Acid					
A2	1028.591	−23.715	−7.286				343.15	373.15	0.081	92-ban/gar
					Dodecanoic Acid					
A2	1016.266	−21.787	−7.285				343.15	373.15	0.054	92-ban/gar
					Tetradecanoic Acid					
A2	1114.020	−76.200					353.15	373.15	0.078	92-ban/gar
					Hexadecanoic Acid					
A2	1109.558	−75.740					353.15	373.15	0.081	92-ban/gar
					Methyl Ethanoate					
A1	1.47530	1.35621			324.910	506.80	253.15	313.15	0.408	78-kum/iwa
					Ethyl Ethanoate					
A1	1.69043	2.64150	−4.70476	3.52368	308.064	523.20	273.15	473.15	0.106	69-trc[i]
					1-Methylethyl Ethanoate					
A2	1298.373	−162.582	6.2022				297.17	367.20	0.000[e]	75-gus/kad
					Propyl Propanoate					
A1	4.99964	−8.04117	6.23552		294.076	571.00	300.00	400.00	1.677	78-gus/kli
					3-Methylbutyl Propanoate					
A2	1100.050	−66.234	−4.333				298.15	423.15	0.157	76-gus/kli
					Methyl Hexanoate					
A2	1170.294	−101.267	0.376				294.99	408.85	0.536	92-mus/gus
					Nonyl Hexanoate					
A2	1248.402	−211.291	36.084	−3.277			289.00	549.37	0.235	92-mus/gus-1
					2-Methylpropyl 2-Hydroxypropanoate					
A2	959.494	38.991	−10.133				294.36	371.42	0.078	91-gus/kul
					Pentyl 2-Hydroxypropanoate					
A2	1178.221	−67.054					296.71	371.82	1.279	91-gus/kul-1
					Methyl Benzenecarboxylate					
A2	1265.729	−38.365	−7.623				300.48	440.59	0.292	94-mus/tag
					2-Ethylhexyl Benzenecarboxylate					
A2	1192.191	−77.500					253.15	373.15	0.000[h]	88-wal/lam
					Methyl 2-Hydroxybenzenecarboxylate					
A1	3.91754	−4.77123	4.28255		336.615	763.00	298.15	498.15	0.178	90-mus/gan-1
					Pentyl 2-Hydroxybenzenecarboxylate					
A2	1288.069	−83.477	−0.009				298.15	573.15	0.195	90-mus/gan-1
					Hexyl 2-Hydroxybenzenecarboxylate					
A2	983.795	−60.237	−0.229				298.15	573.15	0.050	90-mus/gan-1
					Methyl 2-Methyl-2-propenoate					
A2	1101.229	0.316	−18.439				289.34	349.29	0.162	87-gus/bai
					Nonyl 2-Methyl-2-propenoate					
A2	1182.666	−117.059	4.949				292.37	473.43	1.192	89-gus/bai
					Diethyl Butane-1,4-dioate					
A2	1382.302	−126.452	3.541				295.65	347.15	0.000[e]	90-mus/gan-3
					Dipropyl Butane-1,4-dioate					
A2	806.562	196.733	−43.665				288.15	347.95	0.147	90-mus/gan-2
					Dinonyl Butane-1,4-dioate					
A2	1075.179	−55.159	−0.080				298.15	573.15	0.109	91-mus/gan

[a] Taken from 93-cda. [b] [83-ing/gro], [87-hol/goe], and [89-ram/kud]. [c] The data from 78-fig/szw differ significantly from recommended values published in 85-trc. [d] Reference 77-apa/ker presents two values of density at atmospheric pressure only, but compressed-liquid density data are inconsistent with the reference line from 91-trc and thus only original reference values were used for the fit in Table 3. [e] Polynomial interpolation. [f] Data from 71-kor are lower by 0.5 kg·m^{-3} in average. [g] Data from 71-kor are lower by 0.2 kg·m^{-3} in average. [h] The fit of all seven data points reported yielded a straight line. [i] Densities from the source other than that of compressed-liquid data.

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) either were not available in original papers or the values at atmospheric pressure were reported for different temperatures than compressed-liquid density data, 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

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

$$\rho(T/\mathrm{K})/\mathrm{kg{\cdot}m^{-3}} = a_0 + a_1(T/100) + a_2(T/100)^2 + a_3(T/100)^3 \quad \text{(A2)}$$

The values of adjustable parameters a_i obtained by fitting to available data using a weighted least squares method are recorded in Table A1 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. The references to the saturated vapor pressure data, $P_{ref}(T)$, used in eq 1 are also given in Table A1 in those cases when the upper temperature limit, T_{max}, of the corresponding fit in Table 3 is above the normal boiling temperature. It should be pointed out that the fits in Table A1 do not represent a critical evaluation of density data at atmospheric pressure or at saturation (except for the fits of recommended density values taken from the TRC Thermodynamic Tables) which is beyond the scope of the present review. On the other hand, reliable and high-quality experimental data were selected where possible (see, e.g., 3-oxapentane).

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 A1 except for 2,5-dioxaheptane [78-sha/bai] and 4,7,10-trioxatridecane [81-sha/abd] where original reference density values, $\rho(T,P_{ref} = 0.101\ 325$ MPa), were smoothed (Table A1) before the use for fits by eq 1 for respective compressed-liquid density data sets since in those two cases the experimental densities at atmospheric pressure and those for the compressed liquid were reported for different temperatures.

Appendix II

Parameters of Smoothing Functions for Original Reference Density Data. Table A2 summarizes values of adjustable parameters a_i of functions A1 and A2 (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 3 and 4). The functions were not, unlike the equations summarized in Table A1, 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 evaluation of compressed-liquid densities from eq 1.

The fits in Table A2 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 A1 and A2 were not reported in original sources; i.e., relative quantities as relative density, $\rho(T,P)/\rho(T,P_{ref})$, volume ratio, $V(T,P)/V(T,P_{ref})$, or compression, $\{1 - V(T,P)/V(T,P_{ref})\}$, only were presented by researchers.

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