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Densities, Isothermal Compressibilities, and Isobaric Thermal Expansivities of Hexan-2-ol, Octan-1-ol, and Decan-1-ol from (313 to 363) K and Pressures up to 22 MPa

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Compressed liquid densities of hexan-2-ol, octan-1-ol, and decan-1-ol were measured from (313 to 363) K and pressures up to 22 MPa. A vibrating tube densimeter was used to obtain the experimental densities. The uncertainty is estimated to be better than $\pm 0.20\ \mathrm{kg \cdot m^{-3}}$ for the experimental compressed liquid densities in the whole range of reported data. The experimental data were correlated using a short volume explicit equation of 5 parameters and the 11-parameter Benedict−Webb−Rubin−Starling equation of state (BWRS EoS). Comparisons with literature data were made for octan-1-ol and decan-1-ol. Densities of hexan-2-ol at high pressure were not found in the literature. Isothermal compressibilities and isobaric thermal expansivities were calculated using the 5-parameter equation.

Introduction

Compressed liquid densities of 1-alcohols and their corresponding isomers are of interest in the chemical industry.[1−8] Alcohols are used in a wide range of industrial applications involving hydrocarbon or petroleum fluids.[1] For example, they are used as cosurfactants in oil-in-water emulsions,[2] as additives in gasoline to reduce pollution effect,[3] as inhibitors to prevent the precipitation of gas hydrates in pipelines,[4] and as cosolvent in supercritical fluid technology.[5−8] This last application has been used from the extraction of valuable products from natural products.[9] The use of mixtures composed by a supercritical fluid and a liquid solvent is commonly used to manipulate the solubility and selectivity of the supercritical fluid.[5−8] To study and understand the performance of these fluids under operating conditions, experimental property measurements of pure compound and mixtures can offer valuable information from a modeling and fundamental point of view. One of these properties is the density, which is required in many engineering disciplines and to obtain other thermophysical properties. The present work is part of a systematic study[10−15] to obtain density data of alcohols and CO_2 + alcohol mixtures having as the main goal the development of supercritical fluid technology, such as the extraction of capsaicin from *Capsicum annum*.[16] Extensive reviews of published density data sets for 1-alcohols and 2-alcohols at elevated pressures were made by Cibulka et al.[17,18] Their review covers papers up to 1993[17] for 1-alcohols and up to 1997[18] for 2-alcohols. The characteristics of the different sets of data reported in the literature[19−30] covering papers published up to now for octan-1-ol and decan-1-ol are listed in Table 1. No experimental data were found for hexan-2-ol at high pressure. The experimental measurements obtained in this work are correlated using a short empirical equation[31−32] and the Benedict−Webb−Rubin−Starling equation of state (BWRS EoS).[33] Comparisons with literature data were made using density values calculated from the 5-parameter equation using the parameters fitted to our experimental data. Our density measurements were also compared with the correlations for octan-1-ol and decan-1-ol reported by Cibulka and Zikova.[17] The isothermal compressibility and isobaric thermal expansion are determined using the 5-parameter equation with the parameters obtained for each alcohol studied in this work.

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Experimental Section

Materials. Hexan-2-ol ($C_6H_{14}O$, 102.17 $\mathrm{g \cdot mol^{-1}}$, Chemical Abstracts Service Registry No. (CASRN) 626−93-7) was from Aldrich (U.S.A.) with a stated purity of $x = 0.99$. Octan-1-ol ($C_8H_{18}O$, 130.23 $\mathrm{g \cdot mol^{-1}}$, CASRN 111−87-5) was from Aldrich with a stated purity better than $x = 0.99$. Decan-1-ol ($C_{10}H_{22}O$, 158.28 $\mathrm{g \cdot mol^{-1}}$, CASRN 112−30-1) was from Aldrich with a stated purity of $x = 0.99$. The reference fluids for the calibration of the vibrating tube densimeter were water and nitrogen. Water was HPLC grade and was from Aldrich with a stated purity of $x = 0.9995$. Nitrogen was chromatographic grade with a certified volume fraction purity of 0.99998, and it was from Air-Products Infra (México). The three alcohols were stored over a molecular sieve of 3 Å to avoid any moisture. The purities of the three alcohols samples were tested using a gas chromatograph (HP 5890 series II) fitted with a flame ionization detector and a 0.9144 m × 0.003175 m diameter column packed with Chromosorb 101. After drying and distillation of the alcohols, the purities of hexan-2-ol, octan-1-ol, and decan-1-ol were $x =$ 0.994, 0.995, and 0.993, respectively. Liquid compounds were degassed under vacuum and vigorous stirring before they were used to perform density measurements.

Apparatus and Procedure. Densities were measured with an Anton Paar DMA 60/512P vibrating tube densimeter (VTD). The full scale in temperature is from (263.15 to 423.15) K and in pressure from (0 to 70) MPa. The manufacturer specifications about resolution, repeatability, and uncertainty of density are $1 \cdot 10^{-6}$, $1 \cdot 10^{-5}$, and $1 \cdot 10^{-4}\ \mathrm{g \cdot cm^{-3}}$. The VTD requires build and setup of special peripherals. In our case, it was built to determine densities from (313 to 363) K and pressures up to 25 MPa. Details of the apparatus and experimental procedure

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Table 1. Characteristics of Density Data Sets Reported in the Literature for Octan-1-ol and Decan-1-ol at High Pressure

reference	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	sample purity/%
			octan-1-ol			
Apaev et al.[19]	138	283.15	623.15	5.0	78.8	99.62
Altunin and Konikevich[20]	13	298.15	298.15	0.5	200.0	
Matsuo and Makita[21]	34	298.15	348.15	0.1	40.2	97
Uosaki et al.[22]	4	298.15	298.15	50.0	200.0	
Garg et al.[23]	50	323.15	373.15	0.1	10.0	>99.5
Lee et al.[24]	24	298.15	338.15	5.0	30.0	
Dzida[25]	66	293.15	318.15	0.1	50	99
			decan-1-ol			
Kuss[26]	22	298.15	353.15	19.60	137.30	
Mamedov et al.[27]	42	283.00	473.00	9.80	147.00	
Shelkovenko et al.[28]	75	292.29	573.30	1.09	49.14	98
Matsuo and Makita[21]	28	298.15	348.15	1.00	40.20	>99
Apaev and Gylmanov[29]	112	298.15	623.15	5.00	78.80	98.2
Shakverdiev et al.[30]	49	448.15	573.15	0.16	58.41	99
Dzida[25]	47	293.15	318.15	0.1	70	99

Table 2. (p,ρ,T) Data of Hexan-2-ol at Six Different Temperatures

T/K = 313.13		T/K = 323.09		T/K = 333.04		T/K = 342.98		T/K = 352.86		T/K = 362.73	
p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}
1.010	799.26	1.037	791.00	1.055	782.56	1.032	774.05	1.053	765.06	1.075	754.97
2.006	800.05	2.000	791.79	2.007	783.43	2.015	775.01	2.014	766.05	2.006	756.02
2.999	800.83	3.010	792.63	3.005	784.28	3.012	775.95	3.019	767.09	3.018	757.16
4.008	801.59	4.029	793.48	4.007	785.21	4.017	776.87	4.033	768.08	4.034	758.26
4.999	802.35	5.004	794.27	5.015	786.06	5.013	777.79	4.996	769.01	5.016	759.29
5.986	803.12	6.020	795.10	6.009	786.93	6.012	778.72	6.006	770.06	6.066	760.41
7.000	803.86	7.007	795.84	7.006	787.77	7.025	779.62	7.013	771.02	6.998	761.37
8.010	804.64	8.009	796.68	7.998	788.61	8.000	780.47	8.004	771.95	8.041	762.44
9.026	805.38	9.017	797.48	9.006	789.47	9.000	781.35	9.035	772.93	9.014	763.43
10.004	806.09	10.003	798.25	10.004	790.32	9.996	782.25	10.009	773.84	10.001	764.37
11.005	806.84	11.001	799.00	11.007	791.11	11.020	783.12	11.007	774.75	11.026	765.39
12.001	807.56	12.000	799.77	12.012	791.93	11.999	783.92	12.007	775.66	12.000	766.35
13.010	808.28	13.021	800.56	13.003	792.72	12.996	784.76	12.999	776.54	13.010	767.31
14.002	808.98	14.001	801.30	14.008	793.51	14.007	785.60	14.012	777.47	13.999	768.28
14.998	809.67	15.002	802.00	15.005	794.30	15.003	786.41	15.010	778.33	15.006	769.21
16.001	810.39	16.000	802.74	16.001	795.06	16.005	787.17	16.003	779.21	16.006	770.12
17.006	811.08	17.004	803.48	17.006	795.85	17.002	787.98	17.002	780.07	17.005	771.02
18.000	811.70	18.008	804.21	18.010	796.61	18.010	788.76	18.017	780.92	18.000	771.92
19.005	812.39	19.001	804.90	19.002	797.35	19.005	789.49	19.005	781.75	19.003	772.82
20.015	813.10	20.011	805.62	20.000	798.08	20.010	790.27	20.014	782.58	20.017	773.70
21.029	813.74	21.003	806.31	21.000	798.82	21.006	791.00	21.013	783.39	21.006	774.56
22.004	814.40	22.004	807.01	22.004	799.56	22.005	791.75	22.010	784.18	22.010	775.42

used in this work have been described previously.[10−15] The reliability of the experimental density determinations and of the apparatus has been demonstrated in previous papers.[10−15,31,32,34] The measurement circuit consists of the vibrating tube (Hastelloy C-276 U-tube) containing a sample of approximately 1 cm^3. It is connected to a sapphire tube cell, which is used to feed the fluids to the VTD. The experimental procedure has been previously described.[10,11] Temperature calibrations were made using a calibration system (Automatic Systems F300S, U.S.A.) using a 25 Ω reference probe (Rosemount, England, model 162CE; ±0.005 K certified accuracy traceable to the ITS−90 scale). The uncertainty of temperature measurements by the platinum probes was estimated to be ±0.03 K. The pressure measurements were made directly in the equilibrium cell by means of a 25 MPa Sedeme pressure transducer (France). It was calibrated at temperatures from (313 to 363) K at the same conditions of measurements against a dead weight balance (Desgranges & Huot, France, model 5304; accuracy ± 0.005 % full scale). The uncertainty in the pressure measurements is estimated to be ±0.008 MPa. Water and nitrogen were used as the reference fluids as described in the classical method.[35] The reference densities of water and nitrogen were obtained using the equations of state proposed by Wagner and Pruss.[36] and Span et al.,[37] respectively. Calibration procedures of the platinum temperature probes, the pressure transducer, and the VTD are described in previous papers.[10,38] The uncertainty of the experimental liquid densities presented in this work was estimated to be ±0.20 kg·m^{-3}. The estimation of the uncertainty for the experimental densities was made according to a previous paper.[32]

Results and Discussion

Density Measurements. Densities of hexan-2-ol, octan-1-ol, and decan-1-ol were determined at six temperatures from (313 to 363) K and pressures up to 22 MPa, and they are reported in Tables 2, 3, and 4. Densities of hexan-2-ol cover the density range between (754 to 815) kg·m^{-3}, densities of octan-1-ol cover the density range between (795 to 824) kg·m^{-3}, while densities of decan-1-ol cover the density range between (781 to 830) kg·m^{-3}.

For each component the measured densities were correlated with two different models. Because excellent results were obtained for liquid densities in previous papers,[31,32] a short equation of five parameters was used to correlate the densities reported here. This equation is expressed as

$$v/\mathrm{m^3 \cdot kg^{-1}} = \frac{c_1 + c_2 P}{c_3 - (c_4/T + c_5/T^{1/3}) + P} \qquad (1)$$

where v is the specific volume, and c_i is fitted to experimental (p,ρ,T) data.

Table 3. (p,ρ,T) Data of Octan-1-ol at Six Different Temperatures

T/K = 313.14		T/K = 323.09		T/K = 333.05		T/K = 343.03		T/K = 352.89		T/K = 362.77	
p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}
1.004	811.26	1.007	804.26	1.038	797.31	1.049	790.60	1.023	782.71	1.051	775.67
2.019	811.95	2.016	804.97	2.029	798.03	2.003	791.16	2.011	783.55	2.025	776.41
3.000	812.59	3.019	805.70	2.999	798.76	2.981	791.93	3.032	784.42	3.016	777.19
4.020	813.22	4.025	806.40	4.033	799.51	4.017	792.68	4.022	785.42	4.009	778.05
4.995	813.89	5.012	807.07	5.020	800.25	5.000	793.37	5.005	786.18	4.974	778.77
6.000	814.53	6.093	807.82	6.014	800.97	6.005	794.05	6.026	787.13	6.005	779.51
7.007	815.21	7.143	808.56	7.029	801.69	7.018	794.88	7.003	787.90	7.006	780.30
8.012	815.83	8.009	809.12	8.011	802.44	8.104	795.68	8.016	788.71	8.011	780.95
8.994	816.51	8.989	809.77	9.005	803.11	9.014	796.44	9.007	789.47	9.008	781.79
10.014	817.19	10.014	810.47	10.022	803.83	10.022	797.10	10.003	790.22	10.034	782.62
11.007	817.79	11.031	811.14	11.011	804.55	11.028	797.87	11.022	791.00	11.013	783.32
12.000	818.42	12.010	811.82	12.021	805.23	11.997	798.58	12.170	791.78	11.987	784.03
12.997	819.05	13.005	812.44	13.022	805.92	13.030	799.30	13.015	792.51	13.015	784.77
14.001	819.67	14.003	813.11	14.031	806.61	14.005	800.00	14.018	793.24	14.006	785.51
14.997	820.27	15.012	813.76	15.010	807.28	15.002	800.66	15.009	794.00	14.997	786.30
16.002	820.89	16.009	814.40	16.023	807.92	16.032	801.38	16.023	794.74	16.001	787.03
17.001	821.48	17.005	815.04	17.012	808.59	17.016	801.99	17.010	795.48	17.013	787.79
17.997	822.10	18.013	815.66	18.035	809.23	18.012	802.68	18.002	796.16	17.997	788.55
19.004	822.69	19.003	816.26	19.009	809.87	19.005	803.29	19.029	796.90	19.000	789.33
20.007	823.28	20.025	816.90	20.002	810.51	20.018	803.98	20.046	797.63	20.023	790.04
21.004	823.86	21.081	817.56	21.011	811.15	21.014	804.61	21.023	798.30	21.004	790.83
		22.009	818.09	22.019	811.82	22.004	805.23				

Table 4. (p,ρ,T) Data of Decan-1-ol at Six Different Temperatures

T/K = 313.12		T/K = 323.09		T/K = 333.04		T/K = 342.98		T/K = 352.86		T/K = 362.89	
p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}	p/MPa	ρ/kg·m^{-3}
1.025	816.79	1.002	809.87	1.046	802.82	1.058	795.63	1.069	788.44	1.077	781.02
2.002	817.46	2.011	810.59	2.018	803.50	2.045	796.40	2.043	789.24	2.027	781.83
2.995	817.98	3.019	811.21	3.008	804.21	3.022	797.12	3.040	790.04	3.089	782.69
4.013	818.58	4.014	811.83	4.012	804.88	4.035	797.90	4.048	790.78	4.047	783.49
5.004	819.21	5.006	812.47	5.059	805.62	5.028	798.63	5.038	791.59	5.061	784.29
5.994	819.86	6.012	813.18	6.016	806.29	6.030	799.37	6.043	792.34	6.060	785.12
7.003	820.47	7.002	813.80	7.022	807.00	7.023	800.07	7.038	793.09	7.041	785.91
7.997	821.19	8.003	814.42	8.014	807.64	8.028	800.78	8.039	793.84	8.049	786.70
9.000	821.73	9.008	815.10	9.015	808.34	9.062	801.51	9.040	794.57	9.049	787.47
9.994	822.38	10.006	815.70	10.015	808.97	10.035	802.22	10.038	795.32	10.052	788.25
10.995	823.02	11.000	816.38	11.019	809.64	11.029	802.92	11.032	796.04	11.045	788.99
11.995	823.67	12.002	816.97	12.007	810.31	12.064	803.64	12.032	796.74	12.044	789.75
12.997	824.20	13.002	817.64	13.019	810.96	13.023	804.31	13.040	797.47	13.054	790.54
13.996	824.82	14.000	818.21	14.019	811.60	14.042	805.00	14.046	798.18	14.053	791.25
14.998	825.42	15.017	818.84	15.014	812.24	15.022	805.66	15.043	798.89	15.052	792.00
15.990	826.01	16.003	819.40	16.021	812.88	16.022	806.36	16.037	799.59	16.056	792.77
16.995	826.61	17.015	820.02	17.026	813.50	17.021	807.00	17.040	800.26	17.063	793.47
17.986	827.14	18.006	820.61	18.023	814.11	18.034	807.70	18.046	800.95	18.062	794.20
18.992	827.76	19.007	821.24	19.018	814.72	19.025	808.35	19.040	801.63	19.062	794.91
19.993	828.31	20.007	821.84	20.025	815.35	20.038	808.98	20.064	802.32	20.068	795.64
20.999	828.88	21.002	822.41	21.020	815.94	21.018	809.62	21.048	802.96	21.072	796.35
21.509	829.19	22.014	823.01	22.032	816.58	22.035	810.28	22.049	803.62	22.063	797.03

The other equation used to correlate the experimental density data was the BWRS EoS, expressed as[33]

$$p/\mathrm{bar} = \frac{RT}{V_\mathrm{m}} + \frac{(B_0RT - A_0 - C_0/T^2 + D_0/T^3 - E_0/T^4)}{V_\mathrm{m}^{\,2}} + \frac{(bRT - a - d/T)}{V_\mathrm{m}^{\,3}} + \frac{\alpha(a + d/T)}{V_\mathrm{m}^{\,6}} + \frac{c(1 + u/V_\mathrm{m}^{\,2})\exp(-u/V_\mathrm{m}^{\,2})}{V_\mathrm{m}^{\,3}T^2} \qquad (2)$$

where V_m is the molar volume.

The values for the parameters of eqs 1 and 2 were obtained by minimizing the deviations between the model and the experimental densities of the pure fluid using the Marquardt–Levenberg least-squares optimization with the following objective function, S:

$$S = \sum_i \left[\frac{\rho_i(\mathrm{expt}) - \rho_i(\mathrm{calc})}{\rho_i(\mathrm{expt})}\right]^2 \qquad (3)$$

The number of data points (N_p), ranges of temperature, pressure, and density used in the correlations, along with the optimized parameters and statistical values[31,32,34] to evaluate the correlations are presented in Table 5 for the three alcohols studied in this work.

Relative deviations of experimental densities (ρ(exptl)) with values calculated (ρ(calc)) using the BWRS EoS for hexan-2-ol are plotted in Figure 1. The maximum relative deviations are ±0.05 % for the BWRS EoS as depicted in Figure 1. The same maximum deviations were obtained for the 5-parameter equation. Both equations represent the experimental density data of hexan-2-ol with a standard deviation (SDV) of 0.03 %; this value is consistent with the experimental uncertainty declared in this work. The relative deviations of experimental densities of octan-1-ol (ρ(exptl)) with values calculated (ρ(calc)) with the 5-parameter equation are illustrated in Figure 2. The maximum deviation is +0.052 % and the minimum deviation is −0.042 % as can bee seen in Figure 2. For the BWRS EoS, the maximum deviation was +0.048 and the minimum deviation was −0.044. Two equations represent the experimental densities

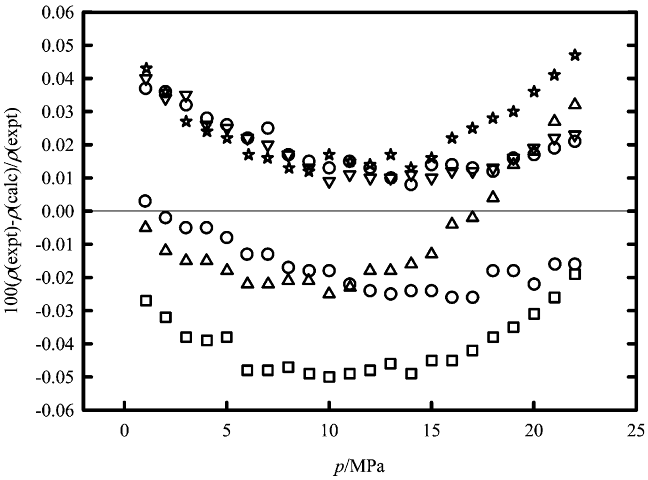

Figure 1. Relative deviations of experimental densities from this work (ρ(expt)) and values calculated (ρ(calc)) with the BWRS EoS using the parameters reported in Table 5 for hexan-2-ol at the following temperatures: ○, 313.13 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.73 K.

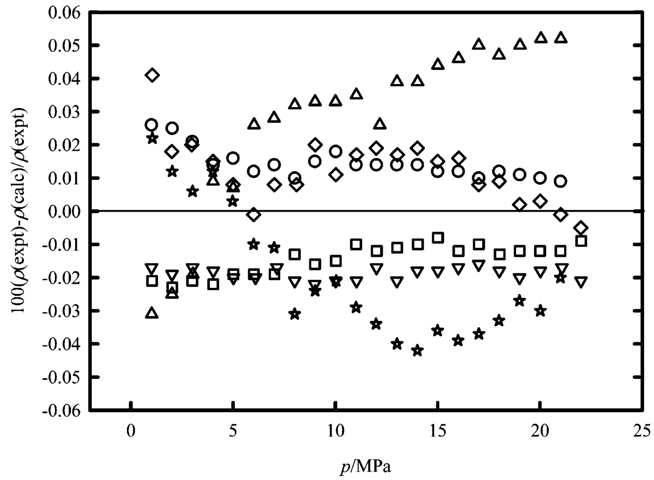

Figure 2. Relative deviations of experimental densities from this work (ρ(expt)) and values calculated (ρ(calc)) with the 5-parameter equation using the parameters reported in Table 5 for octan-1-ol at the following temperatures: ○, 313.14 K; ▽, 323.09 K; □, 333.05 K; ◇, 343.03 K; △, 352.89 K; ☆, 362.77 K.

of octan-1-ol within the experimental uncertainty with the SDV being 0.02 %. In Figure 3, the relative deviations between experimental densities of decan-1-ol and values calculated with the BWRS EoS are shown. The maximum and minimum relative deviations from Figure 3 are −0.017 and +0.014, respectively. Similar deviations were obtained for the 5-parameter equation. These two equations represent the experimental densities of decan-1-ol with a SDV of 0.01 %. In general, the two equations used in this work represent the experimental density within the declared experimental uncertainty.

The consistency of the experimental densities was done by comparing our experimental data (or the correlations obtained) with density data and correlations reported in the literature. No background exists of densities in the literature for hexan-2-ol; the data set presented here represent the first reported at high pressure. Densities of octan-1-ol and of decan-1-ol have been studied before, and the characteristics of the data sets published are summarized in Table 1.

Because no comparison of densities at high pressure was possible, density values of hexan-2-ol at atmospheric pressure calculated with the 5-parameter equation were compared with experimental data reported in the literature.[39−42] The relative deviations of experimental densities from literature (ρ(lit)) with calculated values (ρ(calc)) is depicted in Figure 4. The best

Table 5. Temperature T, Pressure p, and Density ρ Ranges, Data Points N_p, and Parameters for the Two Correlation Models for Hexan-2-ol, Octan-1-ol, and Decan-1-ol along with Statistical Values: AAD, Mean Deviation Bias, SDV, and rms

	hexan-2-ol	octan-1-ol	decan-1-ol
T_{min}/K	313.13	313.14	313.12
T_{max}/K	362.73	362.77	362.89
p_{min}/MPa	1.010	1.004	1.002
p_{max}/MPa	22.010	22.019	22.063
ρ_{min}/kg·m^{-3}	754.97	775.67	781.02
ρ_{max}/kg·m^{-3}	814.40	823.86	829.19
N_p	132	129	132
	5-parameters equation		
c_1/MPa·kg^{-1}·m^3	0.16583	0.24011	0.21512
c_2/kg^{-1}·m^3	0.001081	0.001028	0.001049
c_3/MPa	−437.548	−400.559	−265.660
c4/K·MPa	70257.1	70048.2	47261.2
c_5/MPa·K$^{1/3}$	−5393.7	−5560.4	−4021.0
AAD/%	0.03	0.02	0.005
bias/%	−0.0002	−0.002	0.005
SDV/%	0.03	0.02	0.01
rms/%	0.03	0.02	0.01
	BWRS EoS		
B_0/cm^3·mol^{-1}	664.01	237.78	302.69
A_0/bar·cm^6·mol^{-2}	4.1900·10^7	6.0067·10^7	7.4694·10^7
C_0/bar·K^2·cm^6·mol^{-2}	1.3345·10^{12}	3.5131·10^{12}	4.6815·10^{12}
D_0/bar·K^3·cm^6·mol^{-2}	−2.0618·10^{14}	−4.3430·10^{14}	−5.5842·10^{14}
E_0/bar·K^4·cm^6·mol^{-2}	−1.1622·10^{17}	−2.5917·10^{17}	−2.9681·10^{17}
b/cm^6·mol^{-2}	5.9113·10^4	2.0213·10^5	2.8979·10^5
a/bar·cm^9·mol^{-3}	2.6693·10^8	9.5285·10^8	2.0085·10^9
d/bar·K·cm^9·mol^{-3}	5.2406·10^{10}	4.5534·10^{10}	2.0765·10^{11}
c/bar·K^2·cm^9·mol^{-3}	−3.8020·10^{14}	−6.985·10^{14}	−1.2529·10^{15}
α/cm^9·mol^{-3}	2.3461·10^7	3.9899·10^7	5.7066·10^7
u/cm^6·mol^{-2}	2.4210·10^4	4.9619·10^4	5.7597·10^4
AAD/%	0.02	0.02	0.01
bias/%	−0.0004	−0.0002	−0.0005
SDV/%	0.03	0.02	0.01
rms/%	0.03	0.02	0.01

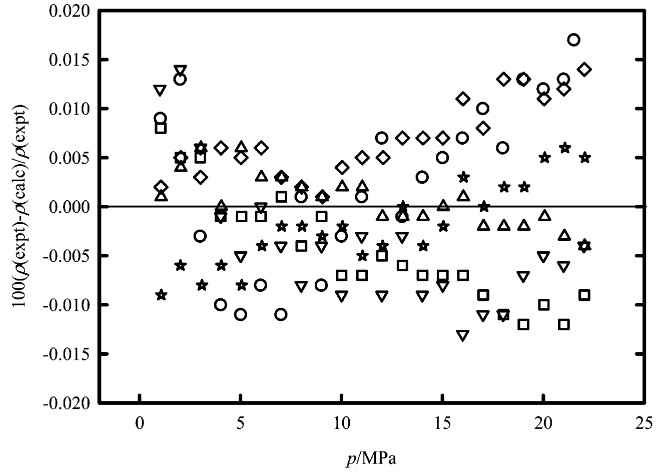

Figure 3. Relative deviations of experimental densities from this work (ρ(expt)) and values calculated (ρ(calc)) with the BWRS EoS using the parameters reported in Table 5 for decan-1-ol at the following temperatures: ○, 313.12 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.89 K.

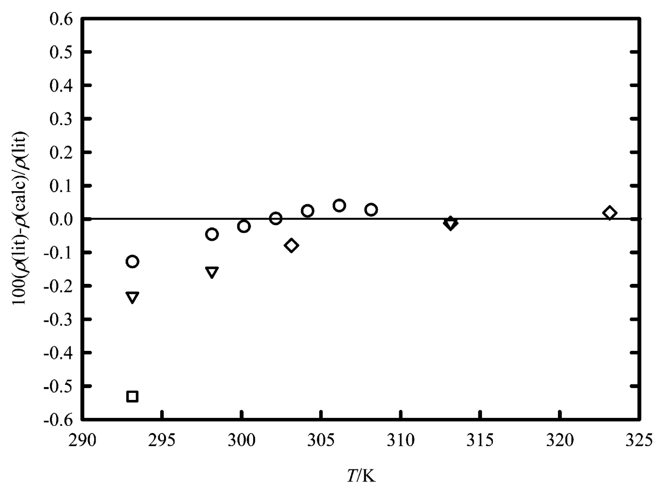

Figure 4. Comparison of experimental densities at atmospheric pressure for hexan-2-ol reported by different authors in the literature (ρ(lit)) with the values calculated from the 5-parameter equation (ρ(calc)) fitted to data reported in this work; ○, Ortega;[39] ▽, TRC Tables;[40] □, Iloukhani et al.;[41] ◇, Weng and Chen.[42]

agreement was found with the data reported by Ortega[39] and Weng and Chen.[42] The 5-parameter equation represents their data with an average absolute deviation (AAD) of 0.04 %. Larger deviations were founded with the data from ref 40 and Iloukhani et al.[41] The deviations increased as the temperature decreases as can be seen in Figure 4.

Cibulka and Zikova[17] reported two different correlations for octan-1-ol. The first correlation was obtained using data reported by Matsuo and Makita,[21] Uoasaki et al.,[22] and Garg et al.[23] (named 1-Octanol (I)), and the second one (1-Octanol (II)) was obtained using the above data along with those reported by Apaev et al.[19] Density values at the same conditions reported herein were calculated with the two mentioned correlations. The relative deviation of experimental data from this work and values calculated with both correlations are shown in Figure 5. The maximum deviations are ±0.08 % for both correlations. No difference is observed for both correlations by observing Figure 5; however, to evaluate this comparison the absolute (rmsd) and relative (rmsdr) root-mean-square deviation, and bias, as defined in ref 17, were calculated for our set of data for both correlations. The results are 0.353 $kg \cdot m^{-3}$, 0.044 %, and 0.002 $kg \cdot m^{-3}$, respectively, for 1-Octanol (I) correlation, and 0.316 $kg \cdot m^{-3}$,

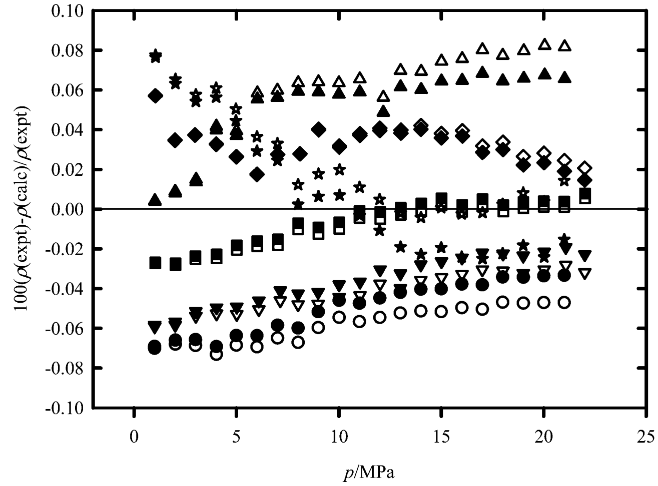

Figure 5. Relative deviations of experimental densities of octan-1-ol from this work (ρ(expt)) and values calculated (ρ(calc)) using the correlations reported by Cibulka and Zikova[17] for octan-1-ol at the following temperatures: ○, 313.14 K; ▽, 323.09 K; □, 333.05 K; ◇, 343.03 K; △, 352.89 K; ☆, 362.77 K. Open and closed symbols are for 1-Octanol (I) and 1-Octanol (II) correlations from ref 17, respectively.

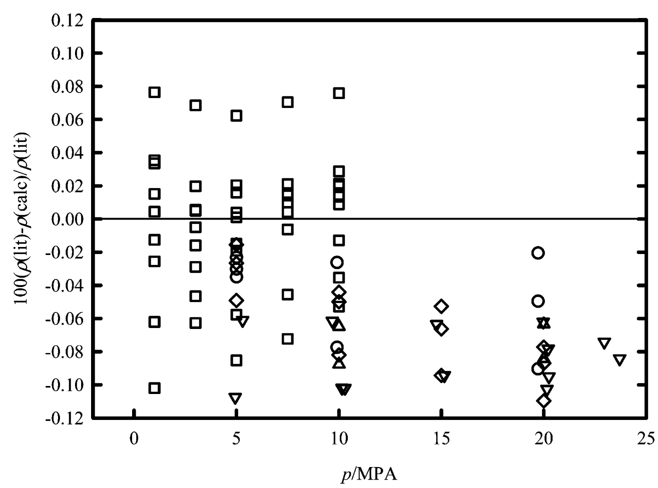

Figure 6. Comparison of the experimental densities at high pressure of octan-1-ol reported by different authors (ρ(lit)) with values calculated from the 5-parameter equation (ρ(calc)) fitted to data reported in this work; ○, Apaev et al.;[19] ▽, Matsuo and Makita;[21] □, Garg et al.;[23] ◇, Lee et al.;[24] △, Dzida.[25]

0.039 %, and −0.005 $kg \cdot m^{-3}$, respectively, for 1-Octanol (II) correlation. The second correlation represents with better accuracy our experimental data, and the statistical values obtained are lower than those obtained for the 1-Octanol (II) correlation.[17] Additionally to this comparison, the 5-parameter equation with the parameters obtained here for octan-1-ol was used to calculate densities at the same temperature and pressure of the data reported in the literature; however, only those data reported in the same range of temperature and pressure measured here were considered. The relative deviations for the different sets of data considered are plotted in Figure 6. The average absolute deviations for individual sets of data compared are 0.04 % (Apaev et al.[19]), 0.08 % (Matsuo and Makita[21]), 0.03 % (Garg et al.[23]), 0.06 % (Lee et al.[24]), and 0.07 % (Dzida[25]). Comparisons of density at atmospheric pressure are shown in Figure 7 for octan-1-ol. Relative deviations of values calculated with the 5-parameter equation for octan-1-ol with density data reported in the literature.[21,23,25,43−46] The maximum deviation is +0.1 % and the minimum deviation is −0.34 % as can be seen in Figure 7. The average absolute deviations for each set of data used in the comparison are as follows: 0.20 % (Diaz-Peña and

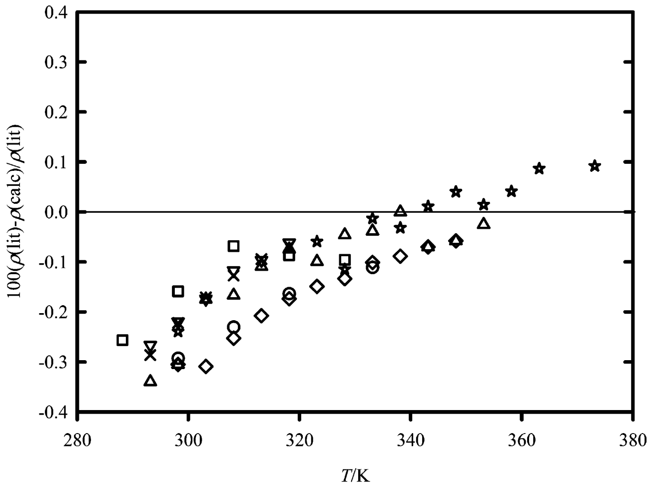

Figure 7. Comparison of experimental densities at atmospheric pressure for octan-1-ol reported in the literature (ρ(lit)) with the values calculated from the 5-parameter equation (ρ(calc)) fitted to data reported in this work; ○, Diaz-Peña and Tardajos;[43] ▽, Ortega;[44] □, Rauf et al.;[45] ◊, Matsuo and Makita;[21] △, Liew et al.;[46] ☆, Garg et al.;[23] ×, Dzida.[25]

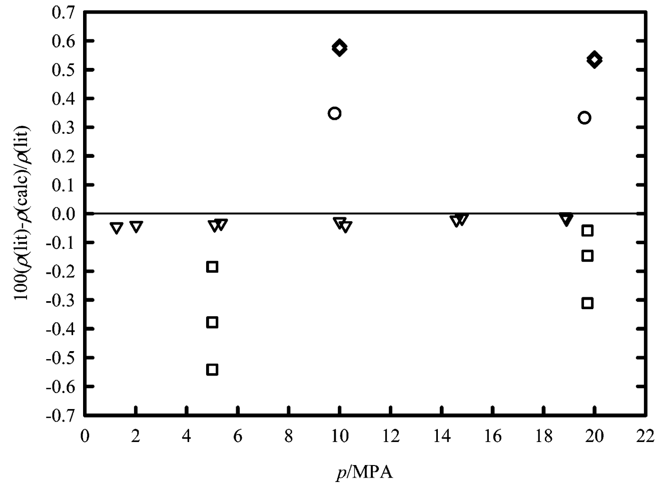

Figure 9. Comparison of the experimental densities at high pressure of decan-1-ol reported by different authors (ρ(lit)) with values calculated from the 5-parameter equation (ρ(calc)) fitted to data reported in this work; ○, Mamedov and Aliev;[27] ▽, Matsuo and Makita;[21] □, Apaev and Gylmanov;[29] ◊, Dzida.[25]

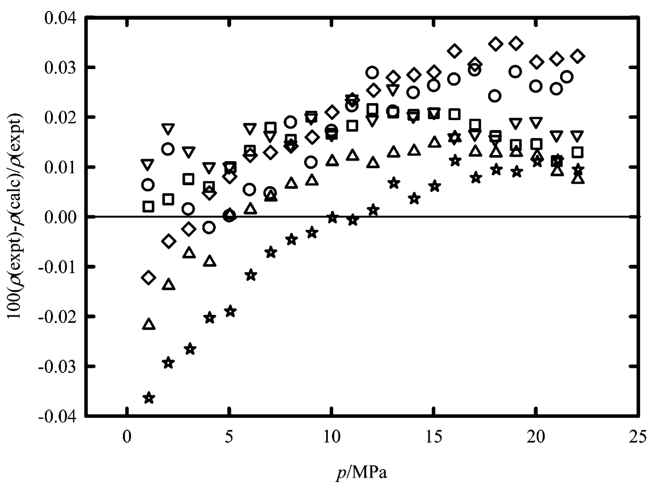

Figure 8. Relative deviations of experimental densities of decan-1-ol from this work (ρ(expt)) and values calculated (ρ(calc)) using the correlation reported by Cibulka and Zikova[17] for decan-1-ol at the following temperatures: ○, 313.12 K; ▽, 323.09 K; □, 333.04 K; ◊, 342.98 K; △, 352.86 K; ☆, 362.89 K.

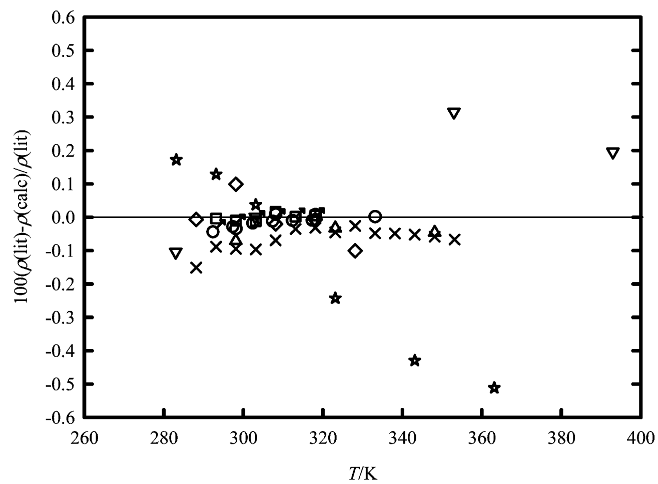

Figure 10. Comparison of experimental densities at atmospheric pressure for decan-1-ol reported by different authors (ρ(lit)) and values calculated with the 5-parameter equation (ρ(calc)) fitted to data reported in this work; ○, Diaz-Peña and Tardajos;[43] ▽, Mamedov and Aliev;[27] □, Ortega;[44] ◊, Rauf et al.;[45] △, Matsuo and Makita;[21] ☆, Apaev and Gylmanov;[29] ×, Liew et al.;[46] ♂, Dzida.[25]

Tardajos[43]), 0.16 % (Ortega[44]), 0.13 % (Rauf et al.[45]), 0.17 % (Matsuo and Makita[21]), 0.12 % (Liew et al.[46]), 0.07 % (Garg et al.[23]), and 0.16 % (Dzida[25]).

For decan-1-ol, we compare our data with the correlation reported by Cibulka and Zikova.[17] This correlation was done using the density data sets reported by Kuss,[26] Matsuo and Makita,[21] and Apaev and Gylmanov.[29] The relative deviations between the experimental data and the model are plotted in Figure 8. The maximum deviations are ±0.04 %. As for the case of octan-1-ol, the rmsd, rmsdr, and bias were calculated for our set of data, and the results are 0.144 $kg \cdot m^{-3}$, 0.018 %, and 0.097 $kg \cdot m^{-3}$. These values are lower compared to the values reported for the correlation.[17] This demonstrates good agreement with the correlation reported by Cibulka and Zikova.[17] The 5-parameter equation with the parameters reported in Table 5 for decan-1-ol was used to calculate density values at the same conditions of temperature and pressure reported in the literature, considering only data reported in the same range of temperature and pressure used in this work. The relative deviations of calculated densities and literature data[21,25,27,29] are shown in Figure 9. The maximum deviations are ±0.6 %, and the best agreement was found with the data reported by Matsuo and Makita,[21] having an AAD of 0.02 % with respect to the model. The AAD values for the remaining sets of data are as follows: 0.31 % (Mamedov and Aliev[27]), 0.26 % (Apaev and Gylmanov[29]), and 0.56 % (Dzida[25]). Comparisons for decan-1-ol at atmospheric pressure were also done, and the relative deviations of density values calculated with the 5-parameter equation with literature data[21,25,27,29,43−46] are shown in Figure 10. Excellent agreement was found with the data reported by Ortega[44] and Dzida[25] having both sets of data with AAD values of 0.01 % with respect to the model. For the other sets of data, the AAD values are 0.12 % (Diaz-Peña and Tardajos[43]), 0.11 % (Mamedov and Aliev[27]), 0.04 % (Rauf et al.[45]), 0.05 % (Matsuo and Makita[21]), 0.25 % (Apaev and Gylmanov[29]), and 0.05 % (Liew et al.[46]). The different comparisons show the reliability of our experimental data.

Derived Properties. The experimental densities can be used to obtain some thermodynamic properties, such as the isothermal compressibility (K_T) and the isobaric thermal expansivity (α_p). The effect of pressure in density can be described by the

Table 6. Calculated Values of Isothermal Compressibility, K_T, and Isobaric Thermal Expansivity, α_p, for Hexan-2-ol

T = 313.13 K			T = 323.09 K			T = 333.04 K			T = 342.98 K			T = 352.86 K			T = 362.73 K		
p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$
MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}
1.010	1.021	0.967	1.037	1.096	1.044	1.055	1.178	1.113	1.032	1.266	1.174	1.053	1.358	1.228	1.075	1.455	1.277
2.006	1.007	0.960	2.000	1.082	1.037	2.007	1.162	1.104	2.015	1.248	1.165	2.014	1.339	1.219	2.006	1.435	1.267
2.999	0.993	0.953	3.010	1.067	1.029	3.005	1.146	1.096	3.012	1.231	1.156	3.019	1.320	1.209	3.018	1.415	1.257
4.008	0.980	0.946	4.029	1.052	1.021	4.007	1.130	1.088	4.017	1.214	1.147	4.033	1.302	1.200	4.034	1.395	1.247
4.999	0.967	0.939	5.004	1.038	1.014	5.015	1.115	1.080	5.013	1.197	1.139	4.996	1.284	1.191	5.016	1.376	1.238
5.986	0.954	0.932	6.020	1.023	1.006	6.009	1.100	1.072	6.012	1.181	1.130	6.006	1.266	1.182	6.066	1.356	1.228
7.000	0.941	0.926	7.007	1.010	0.999	7.006	1.085	1.064	7.025	1.164	1.122	7.013	1.249	1.173	6.998	1.338	1.219
8.010	0.928	0.919	8.009	0.996	0.992	7.998	1.070	1.056	8.000	1.149	1.114	8.004	1.232	1.164	8.041	1.319	1.210
9.026	0.916	0.912	9.017	0.983	0.985	9.006	1.056	1.049	9.000	1.134	1.106	9.035	1.215	1.156	9.014	1.302	1.201
10.004	0.904	0.906	10.003	0.970	0.978	10.004	1.042	1.041	9.996	1.119	1.098	10.009	1.199	1.147	10.001	1.284	1.192
11.005	0.892	0.900	11.001	0.958	0.971	11.007	1.028	1.034	11.020	1.104	1.089	11.007	1.183	1.139	11.026	1.267	1.183
12.001	0.881	0.894	12.000	0.945	0.964	12.012	1.015	1.026	11.999	1.089	1.082	12.007	1.168	1.131	12.000	1.250	1.175
13.010	0.869	0.887	13.021	0.933	0.957	13.003	1.002	1.019	12.996	1.075	1.074	12.999	1.152	1.123	13.010	1.234	1.166
14.002	0.858	0.881	14.001	0.921	0.951	14.008	0.989	1.012	14.007	1.061	1.067	14.012	1.137	1.115	13.999	1.218	1.158
14.998	0.848	0.875	15.002	0.909	0.944	15.005	0.976	1.005	15.003	1.047	1.059	15.010	1.123	1.107	15.006	1.202	1.150
16.001	0.837	0.869	16.000	0.898	0.938	16.001	0.964	0.998	16.005	1.034	1.052	16.003	1.108	1.099	16.006	1.186	1.142
17.006	0.826	0.864	17.004	0.886	0.932	17.006	0.951	0.992	17.002	1.021	1.045	17.002	1.094	1.092	17.005	1.171	1.133
18.000	0.816	0.858	18.008	0.875	0.925	18.010	0.939	0.985	18.010	1.008	1.037	18.017	1.080	1.084	18.000	1.156	1.126
19.005	0.806	0.852	19.001	0.865	0.919	19.002	0.928	0.978	19.005	0.995	1.030	19.005	1.066	1.077	19.003	1.141	1.118
20.015	0.796	0.847	20.011	0.854	0.913	20.000	0.916	0.972	20.010	0.983	1.023	20.014	1.053	1.069	20.017	1.127	1.110
21.029	0.786	0.841	21.003	0.843	0.907	21.000	0.905	0.965	21.006	0.971	1.017	21.013	1.040	1.062	21.006	1.113	1.102
22.004	0.777	0.836	22.004	0.833	0.901	22.004	0.894	0.959	22.005	0.959	1.010	22.010	1.027	1.055	22.010	1.099	1.095

Table 7. Calculated Values of Isothermal Compressibility, K_T, and Isobaric Thermal Expansivity, α_p, for Octan-1-ol

T = 313.14 K			T = 323.09 K			T = 333.05 K			T = 343.03 K			T = 352.89 K			T = 362.77 K		
p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$
MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}
1.004	0.850	0.804	1.007	0.892	0.851	1.038	0.937	0.891	1.049	0.984	0.926	1.023	1.033	0.957	1.051	1.084	0.984
2.019	0.842	0.800	2.016	0.884	0.846	2.029	0.928	0.886	2.003	0.975	0.922	2.011	1.024	0.952	2.025	1.074	0.979
3.000	0.834	0.796	3.019	0.876	0.842	2.999	0.920	0.882	2.981	0.966	0.917	3.032	1.014	0.947	3.016	1.064	0.974
4.020	0.826	0.792	4.025	0.867	0.838	4.033	0.911	0.877	4.017	0.957	0.912	4.022	1.004	0.942	4.009	1.054	0.969
4.995	0.819	0.788	5.012	0.860	0.833	5.020	0.903	0.873	5.000	0.948	0.908	5.005	0.995	0.938	4.974	1.044	0.964
6.000	0.812	0.784	6.093	0.851	0.829	6.014	0.894	0.868	6.005	0.939	0.903	6.026	0.986	0.933	6.005	1.034	0.959
7.007	0.804	0.780	7.143	0.843	0.824	7.029	0.886	0.864	7.018	0.931	0.898	7.003	0.977	0.928	7.006	1.025	0.954
8.012	0.797	0.776	8.009	0.836	0.821	8.011	0.878	0.860	8.104	0.921	0.893	8.016	0.968	0.923	8.011	1.015	0.949
8.994	0.790	0.773	8.989	0.829	0.817	9.005	0.870	0.855	9.014	0.914	0.889	9.007	0.959	0.918	9.008	1.006	0.944
10.014	0.783	0.769	10.014	0.821	0.813	10.022	0.862	0.851	10.022	0.905	0.885	10.003	0.950	0.914	10.034	0.996	0.939
11.007	0.776	0.765	11.031	0.814	0.809	11.011	0.854	0.847	11.028	0.897	0.880	11.022	0.941	0.909	11.013	0.987	0.935
12.000	0.769	0.761	12.010	0.807	0.805	12.021	0.847	0.843	11.997	0.889	0.876	12.170	0.932	0.904	11.987	0.979	0.930
12.997	0.762	0.758	13.005	0.799	0.801	13.022	0.839	0.839	13.030	0.881	0.872	13.015	0.924	0.900	13.015	0.970	0.925
14.001	0.755	0.754	14.003	0.792	0.797	14.031	0.832	0.835	14.005	0.873	0.867	14.018	0.916	0.896	14.006	0.961	0.921
14.997	0.749	0.750	15.012	0.785	0.793	15.010	0.824	0.831	15.002	0.866	0.863	15.009	0.908	0.891	14.997	0.952	0.916
16.002	0.742	0.747	16.009	0.778	0.789	16.023	0.817	0.827	16.032	0.858	0.859	16.023	0.900	0.887	16.001	0.944	0.911
17.001	0.736	0.743	17.005	0.772	0.786	17.012	0.810	0.823	17.016	0.850	0.855	17.010	0.892	0.883	17.013	0.935	0.907
17.997	0.729	0.740	18.013	0.765	0.782	18.035	0.803	0.819	18.012	0.843	0.851	18.002	0.884	0.878	17.997	0.927	0.903
19.004	0.723	0.736	19.003	0.758	0.778	19.009	0.796	0.815	19.005	0.836	0.847	19.029	0.876	0.874	19.000	0.919	0.898
20.007	0.717	0.733	20.025	0.752	0.775	20.002	0.789	0.811	20.018	0.828	0.843	20.046	0.868	0.870	20.023	0.911	0.894
21.004	0.711	0.730	21.081	0.745	0.771	21.011	0.782	0.807	21.014	0.821	0.839	21.023	0.861	0.866	21.004	0.903	0.889
			22.009	0.739	0.767	22.019	0.775	0.803	22.004	0.814	0.835						

isothermal compressibility that is calculated using the isothermal pressure derivative of density according to the following expression:

$$K_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial p}\right)_T \tag{4}$$

In this work, the isothermal compressibility of each compound has been determined analytically by differentiating eq 1 along with the parameters reported in Table 5. This results in the following expression for the isothermal compressibility:

$$K_T = \frac{1}{(c_3 - c_4/T - c_5/T^{1/3} + p)} - \frac{c_2}{(c_1 + c_2 p)} \tag{5}$$

The isobaric thermal expansivity is defined as

$$\alpha_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \tag{6}$$

as it was done for the isothermal compressibility. Equation 1, along with the parameters reported in Table 5, is used to derive the isobaric thermal expansivity, obtaining the following expression

$$\alpha_p = -\frac{3c_4/T^2 + c_5/T^{4/3}}{3(c_3 - c_4/T - c_5/T^{1/3} + p)} \tag{7}$$

The uncertainties of the calculated isothermal compressibilities and the calculated isobaric thermal expansivities were calculated with the law of propagation of errors.[47] The uncertainty was

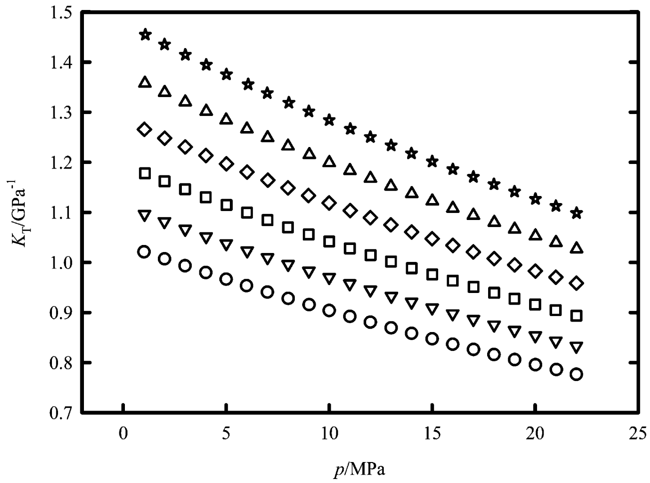

Figure 11. Isotherms for the isothermal compressibility of hexan-2-ol at the following temperatures: ○, 313.13 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.73 K.

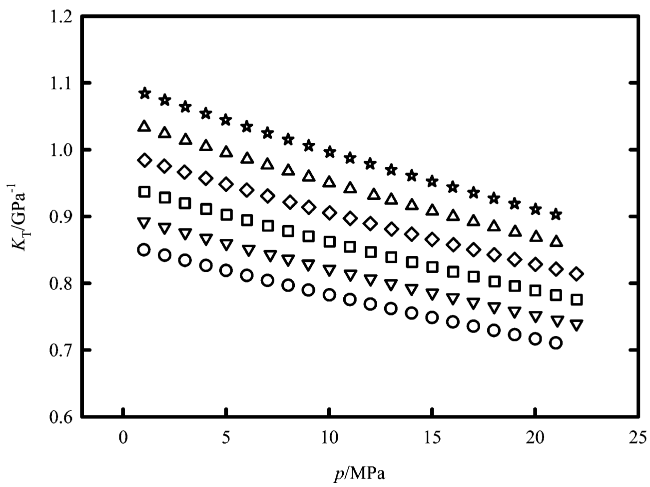

Figure 12. Isotherms for the isothermal compressibility of octan-1-ol at the following temperatures: ○, 313.14 K; ▽, 323.09 K; □, 333.05 K; ◇, 343.03 K; △, 352.89 K; ☆, 362.77 K.

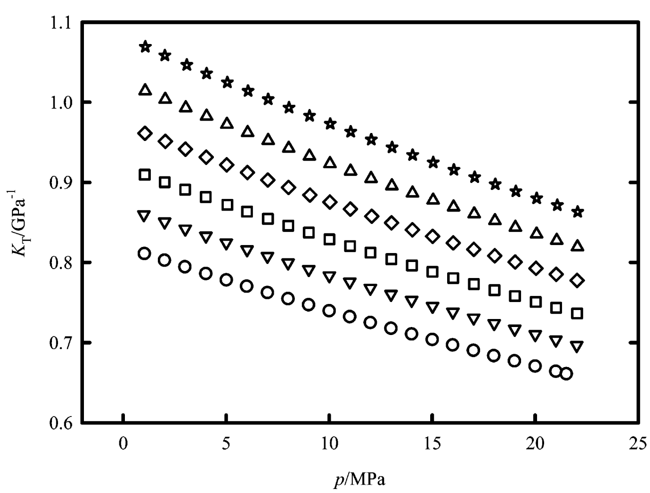

Figure 13. Isotherms for the isothermal compressibility of decan-1-ol at the following temperatures: ○, 313.12 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.89 K.

estimated to be better than ±1.6 % for the isothermal compressibilities, while, the uncertainty for the isobaric thermal expansivities was estimated to be better than ±0.8 %.

The uncertainty on the calculation of the derived thermodynamic properties was obtained based on the next expression for the law of propagation of errors[47]

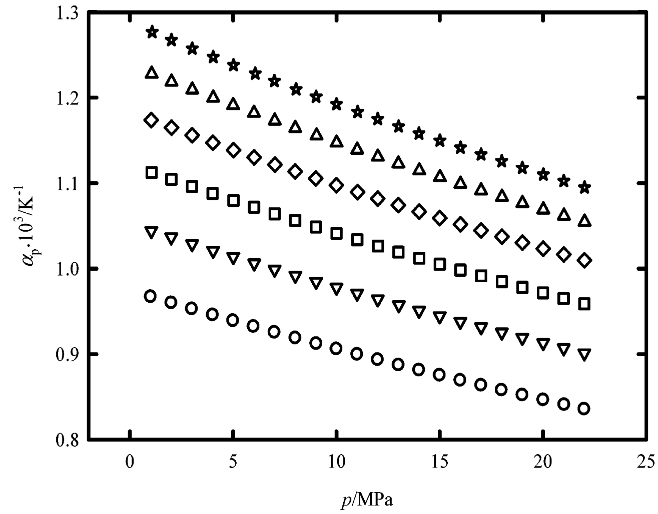

Figure 14. Isotherms for the isobaric thermal expansivity of hexan-2-ol at the following temperatures: ○, 313.13 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.73 K.

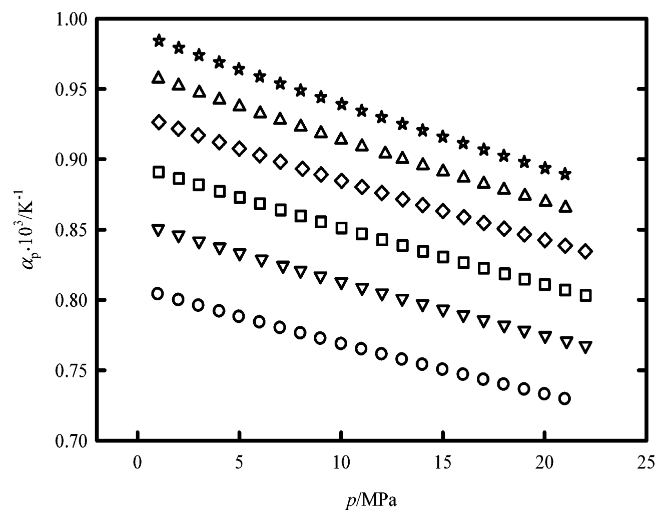

Figure 15. Isotherms for the isobaric thermal expansivity of octan-1-ol at the following temperatures: ○, 313.14 K; ▽, 323.09 K; □, 333.05 K; ◇, 343.03 K; △, 352.89 K; ☆, 362.77 K.

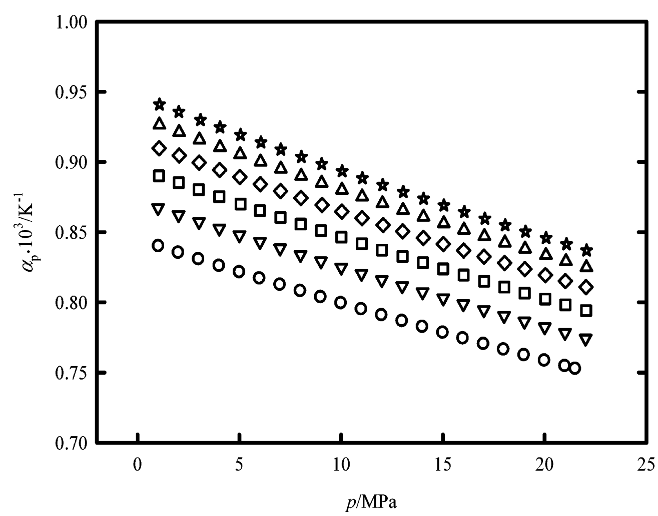

Figure 16. Isotherms for the isobaric thermal expansivity of decan-1-ol at the following temperatures: ○, 313.12 K; ▽, 323.09 K; □, 333.04 K; ◇, 342.98 K; △, 352.86 K; ☆, 362.89 K.

$$\sigma_{K_T}^2 = \sum_{i=1}^{N_p} \left(\frac{\partial K_T}{\partial X_i}\right)^2 \sigma_{X_i}^2 \qquad (8)$$

where the X_i values are referred to as sensitivity coefficients and σ_{X_i} is the standard uncertainty associated with each X_i. For the case of the isothermal compressibility, the following expressions were used:

$$\sigma_{KT}{}^2 = \left(\frac{\partial K_T}{\partial T}\right)^2 \sigma_T^2 + \left(\frac{\partial K_T}{\partial p}\right)^2 \sigma_p^2 + \left(\frac{\partial K_T}{\partial \rho}\right)^2 \sigma_\rho^2 \qquad (9)$$

The derivates with respect to temperature, pressure, and density are given by the following equations:

$$\frac{\partial K_T}{\partial T} = -\left[\frac{3c_4/T^2 + c_5/T^{4/3}}{3(c_3 - c_4/T - c_5 T^{1/3} + p)^2}\right] \qquad (10)$$

$$\frac{\partial K_T}{\partial p} = \frac{-1}{(c_3 - c_4/T - c_5/T^{1/3} + p)^2} + \frac{c_2}{(c_1 + c_2 p)^2} \qquad (11)$$

$$\frac{\partial K_T}{\partial \rho} = \left[\frac{-1}{(c_3 - c_4/T - c_5/T^{1/3} + p)^2} + \frac{c_2}{(c_1 + c_2 p)^2}\right] \left[\frac{(c_1 + c_2 p)^2}{(c_1 + c_2 p) - c_2(c_3 - c_4/T - c_5/T^{1/3} + p)}\right] \qquad (12)$$

On the other hand, for the isobaric thermal expansivity the following expressions were used:

$$\sigma_{\alpha_p}^2 = \left(\frac{\partial \alpha_p}{\partial T}\right)^2 \sigma_T^2 + \left(\frac{\partial \alpha_p}{\partial p}\right)^2 \sigma_p^2 + \left(\frac{\partial \alpha_p}{\partial \rho}\right)^2 \sigma_\rho^2 \qquad (13)$$

The respective derivates are given by the following equations:

$$\frac{\partial \alpha_p}{\partial T} = \frac{3(c_3 - c_4/T - c_5/T^{1/3} + p)(6c_4/T^{-3} - 4c_5/T^{7/3}) + (3c_4/T^2 + c_5/T^{4/3})^2}{9(c_3 - c_4/T - c_5/T^{1/3} + p)^2} \qquad (14)$$

$$\frac{\partial \alpha_p}{\partial p} = \frac{3c_4/T^2 + c_5/T^{4/3}}{3(c_3 - c_4/T - c_5/T^{1/3} + p)^2} \qquad (15)$$

$$\frac{\partial \alpha_p}{\partial \rho} = \left[\frac{3c_4/T^2 + c_5/T^{4/3}}{3(c_3 - c_4/T - c_5/T^{1/3} + p)^2}\right] \left[\frac{(c_1 + c_2 p)^2}{(c_1 + c_2 p) - c_2(c_3 - c_4/T - c_5/T^{1/3} + p)}\right] \qquad (16)$$

Even when the expressions given in eqs 5 and 7 have no explicit dependence on density, the quantities are sensitive to the experimental uncertainty.

The calculated isothermal compressibilities and isobaric thermal expansivities of hexan-2-ol, octan-1-ol, and decan-2-ol calculated with the 5-parameter equation are reported in Tables 6 to 8. The isothermal compresibilities for hexan-2-ol, octan-1-ol, and decan-1-ol are plotted in Figures 11 to 13. K_T increases as the temperature was increased at constant pressure; on the other hand, K_T decreases as the pressure was increased at constant temperature. These two effects can be seen in Figures 11 to 13 for the three alcohols studied here. The alcohols studied in this work become more compressible with increasing temperatures. In contrast, the alcohols become less compressible with increasing pressure. For hexan-2-ol, the isothermal compressibilities range from 1.021 GPa^{-1} at 313.13 K to 1.455 GPa^{-1} at 362.73 K at approximately 1 MPa. For octan-1-ol, the isothermal compressibilities range from 0.850 GPa^{-1} at 313.14 K to 1.084 GPa^{-1} at 362.77 K at approximately 1 MPa. Meanwhile, for decan-1-ol the isothermal compressibilities range from 0.811 GPa^{-1} at 313.12 K to 1.069 GPa^{-1} at 362.89 K at approximately 1 MPa.

The isobaric thermal expansivities for hexan-2-ol, octan-1-ol, and decan-1-ol are plotted in Figures 14 to 16. The isobaric thermal expansivity follows similar behavior of K_T. α_p increases as the temperature was increased at constant pressure. On the other hand, α_p decreases as the pressure was increased at constant temperature, as is depicted in Figures 14 to 16 for hexan-2-ol, octan-1-ol, and decan-1-ol. For hexan-2-ol, the isobaric thermal expansivities range from 0.967 K^{-1} at 313.13

Table 8. Calculated Values of Isothermal Compressibility, K_T, and Isobaric Thermal Expansivity, α_p, for Decan-1-ol

T = 313.12 K			T = 323.09 K			T = 333.04 K			T = 342.98 K			T = 352.86 K			T = 362.89 K		
p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$	p	K_T	$\alpha_p \cdot 10^3$
MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}	MPa	GPa^{-1}	K^{-1}
1.025	0.811	0.840	1.002	0.860	0.867	1.046	0.910	0.890	1.058	0.961	0.910	1.069	1.014	0.926	1.077	1.069	0.941
2.002	0.803	0.835	2.011	0.851	0.862	2.018	0.900	0.885	2.045	0.951	0.905	2.043	1.004	0.921	2.027	1.058	0.936
2.995	0.795	0.831	3.019	0.842	0.857	3.008	0.891	0.880	3.022	0.941	0.900	3.040	0.993	0.916	3.089	1.046	0.930
4.013	0.786	0.826	4.014	0.833	0.853	4.012	0.882	0.875	4.035	0.931	0.894	4.048	0.982	0.911	4.047	1.036	0.925
5.004	0.778	0.822	5.006	0.825	0.848	5.059	0.872	0.870	5.028	0.922	0.889	5.038	0.972	0.905	5.061	1.025	0.919
5.994	0.770	0.817	6.012	0.816	0.843	6.016	0.863	0.865	6.030	0.912	0.884	6.043	0.962	0.900	6.060	1.014	0.914
7.003	0.762	0.813	7.002	0.808	0.839	7.022	0.855	0.861	7.023	0.903	0.879	7.038	0.952	0.895	7.041	1.004	0.909
7.997	0.755	0.808	8.003	0.800	0.834	8.014	0.846	0.856	8.028	0.894	0.874	8.039	0.942	0.890	8.049	0.993	0.904
9.000	0.747	0.804	9.008	0.791	0.829	9.015	0.837	0.851	9.062	0.884	0.869	9.040	0.933	0.885	9.049	0.983	0.899
9.994	0.740	0.799	10.006	0.783	0.825	10.015	0.829	0.846	10.035	0.875	0.865	10.038	0.923	0.880	10.052	0.973	0.893
10.995	0.732	0.795	11.000	0.776	0.820	11.019	0.820	0.842	11.029	0.867	0.860	11.032	0.914	0.875	11.045	0.963	0.888
11.995	0.725	0.791	12.002	0.768	0.816	12.007	0.812	0.837	12.064	0.858	0.855	12.032	0.905	0.870	12.044	0.953	0.884
12.997	0.718	0.787	13.002	0.760	0.812	13.019	0.804	0.833	13.023	0.849	0.851	13.040	0.896	0.866	13.054	0.944	0.879
13.996	0.711	0.783	14.000	0.753	0.807	14.019	0.796	0.828	14.042	0.841	0.846	14.046	0.887	0.861	14.053	0.934	0.874
14.998	0.704	0.778	15.017	0.745	0.803	15.014	0.788	0.824	15.022	0.833	0.841	15.043	0.878	0.856	15.052	0.925	0.869
15.990	0.697	0.774	16.003	0.738	0.799	16.021	0.781	0.819	16.022	0.824	0.837	16.037	0.869	0.852	16.056	0.916	0.864
16.995	0.690	0.770	17.015	0.731	0.795	17.026	0.773	0.815	17.021	0.816	0.833	17.040	0.861	0.847	17.063	0.906	0.860
17.986	0.684	0.766	18.006	0.724	0.790	18.023	0.765	0.811	18.034	0.808	0.828	18.046	0.852	0.843	18.062	0.898	0.855
18.992	0.677	0.762	19.007	0.717	0.786	19.018	0.758	0.807	19.025	0.801	0.824	19.040	0.844	0.838	19.062	0.889	0.850
19.993	0.671	0.759	20.007	0.710	0.782	20.025	0.751	0.802	20.038	0.793	0.819	20.064	0.835	0.834	20.068	0.880	0.846
20.999	0.664	0.755	21.002	0.703	0.778	21.020	0.744	0.798	21.018	0.785	0.815	21.048	0.828	0.829	21.072	0.871	0.841
21.509	0.661	0.753	22.014	0.697	0.774	22.032	0.736	0.794	22.035	0.778	0.811	22.049	0.820	0.825	22.063	0.863	0.837

K to 1.277 K^{-1} at 362.73 K at approximately 1 MPa. The isobaric thermal expansivities for octan-1-ol range from 0.804 K^{-1} at 313.14 K to 0.984 K^{-1} at 362.77 K at approximately 1 MPa. Meanwhile, for decan-1-ol the isobaric thermal expansivities range from 0.840 K^{-1} at 313.12 K to 0.941 K^{-1} at 362.89 K at approximately 1 MPa.

Conclusions

Compressed liquid densities of hexan-2-ol, octan-1-ol, and decan-1-ol were reported at temperatures from (313 to 363) K and pressures up to 22 MPa. New experimental liquid densities for hexan-2-ol were reported at high pressure. These sets of data represent the first reported in the literature for hexan-2-ol at pressures higher than 0.1 MPa. Two equations were used to successfully correlate the experimental density data. Both equations were capable to correlate the reported densities for each alcohol within the experimental uncertainty. The obtained densities (or correlations) of octan-1-ol and decan-1-ol were compared with literature data and available correlations. Good agreement was found with literature data in the ranges of temperature and pressure measured. The extrapolation at atmospheric pressure was in good agreement with selected data published in the literature for the three alcohols. The isothermal compresibilities and isobaric thermal expansivities were calculated with the 5-parameter equation. The uncertainties of these derived properties were estimated to be better than ±1.6 % and ±0.8 %. The influence of temperature and pressure on these properties was discussed.

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