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Compressed Liquid Densities of 1-Pentanol and 2-Pentanol from 313 to 363 K at Pressures to 25 MPa

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Compressed liquid densities of 1-pentanol and 2-pentanol have been measured from 313 to 363 K at pressures to 25 MPa. Measurements have been achieved using a vibrating tube densimeter. Water and nitrogen are the reference fluids to calibrate the densimeter. Measurements uncertainties are estimated to be ±0.03 K for temperatures, ±0.008 MPa for pressures and $\pm 0.20\,\text{kg}\cdot\text{m}^{-3}$ for densities. Two volume-explicit equations with five and six parameters and the 11-parameter BWRS equation of state are used to correlate the experimental densities of 1-pentanol and 2-pentanol reported in this work. Statistical values for the evaluation of the correlations are reported. Comparisons with literature data are performed for the temperature and pressure ranges of the measurements.

KEY WORDS: BWRS EoS; correlation; density; 1-pentanol; 2-pentanol; vibrating tube densimeter.

1. INTRODUCTION

Accurate *PvT* properties of pure compounds are required to develop and test equations of state (EoS). Good correlation and prediction of densities of pure compounds are obtained using multiparameter EoS [1] and volume-explicit expressions [2,3]. These last expressions can be implemented easily, and their practical use is of great significance in the chemical industry; however, the evaluation of experimental density measurements, and perhaps any experimental measurements [4], has become of high

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Table I. Density Data Reported for 1-Pentanol and 2-Pentanol at High Pressure in the Literature

Reference	n	$T_{\min}(K)$	$T_{\max}(K)$	$P_{\min}(MPa)$	$P_{\max}(MPa)$	Compound purity (%)
1-pentanol						
Bridgman [8]	18	298.15	348.15	980.6	4903.3	
Walsh and Rice [9]	2	292.15	296.15	5090	11590	
Sahli et al. [10]	14	293.15	298.15	1	7	99.9
Gylmanov et al. [11]	97	292.30	499.50	0.098	58.80	99.5
Zolin et al. [12]	126	233.13	602.45	1.087	49.14	>99.9
Altunin and Konikevich [13]	13	298.15		0.5	200.0	
Garg et al. [14]	60	323.15	373.15	0.1	10.0	>99 mol
Wappmann et al. [15]	87	228.80	433.00	10.0	200.0	>99
Sülzner and Luft [16]	15	298.15	373.15	50.0	195.0	
2-pentanol						
Sahli et al. [10]	14	293.15	298.15	1	7	99.9
Wappmann et al. [15]	89	234	433	10.000	200.00	>99

importance in the scientific community. Recently, NIST and IUPAC have conducted evaluations of density measurements [5,6]. Cibulka and Ziková [6,7] did a critical evaluation of experimental data for liquid densities of 1-alkanols and 2-alkanols. Their review covered papers published until 1993 for methanol to 1-decanol [6], and for 2-pentanol the revision included papers published up to 1997 [7]. Liquid densities for 1-pentanol at high pressure have been measured by Bridgman [8], Walsh and Rice [9], Sahli et al. [10], Gylmanov et al. [11], Zolin et al. [12], Altunin and Konikevich [13], Garg et al. [14], Wappmann et al. [15], and Sülzner and Luft [16]; however, for 2-pentanol only the experimental densities by Sahli et al. [10] and Wappmann et al. [15] are reported in the literature. The number of data points (n), range of temperature and pressure, and compound purity for the data reported by the mentioned references are presented in Table I.

We report densities for 1-pentanol and 2-pentanol in this work, as a continuation of a systematic study of phase equilibria and density measurements of alkanols and CO_2 + alkanols mixtures [17–24] for supercritical fluid technology applications. Uncertainties for the different measurements are reported according to the most recent recommendations in the literature [4]. All the correlations are reported along with statistical values in order to evaluate the three equations used.

2. EXPERIMENTAL

2.1. Materials

1-pentanol ($C_5H_{12}O$, molar mass = 88.15 g·mol^{-1}, CAS-RN: 71-41-0), and 2-pentanol ($C_5H_{12}O$, molar mass = 88.15 g·mol^{-1}, CAS-RN: 6032-29-7) are from Aldrich (USA) with purities of $>$ 99 mol% and $>$ 98 mol%, respectively. Reference fluids for the calibration of the densimeter are water and nitrogen. Water (HPLC grade, >99.95 mol%) is from Aldrich (USA), and nitrogen (chromatographic grade, 99.995 vol%) is from Air Products-Infra (México). In order to remove any residual moisture, 1-pentanol and 2-pentanol are stored over 3 Å molecular sieves. Water, 1-pentanol, and 2-pentanol were degassed under vacuum and vigorously stirred before they were used.

2.2. Apparatus

The experimental apparatus was previously described [22–27]. It is based on the vibrating tube densimeter (VTD). An Anton Paar DMA 512P VTD was used to determine the density. The full range in temperature is 263.15–423.15 K and in pressure it is 0–70 MPa. A schematic diagram of the experimental apparatus is presented in Fig. 1. The VTD (Hastelloy C-276 U-tube) containing a sample of approximately 1 cm^3 is filled by means of a sapphire tube cell (EC), which allows measurements up to 25 MPa. Pressure measurements are made inside the EC using a pressure transducer (PT) (Sedeme 250, France). Three platinum probes (PTP*i*) (Specitec, France) located in the top and bottom of EC and inserted into the VTD are used for temperature measurements. The VTD is thermoregulated using a circulation liquid bath with water as the refrigerant fluid.

2.3. Experimental Procedures

The apparatus and experimental procedures have been tested previously with different fluids (1-propanol, 2-propanol, decane, *N*, *N*-dimethylformamide, and thiophene) and fluid mixtures (CO_2 + ethanol, 1-propanol, 2-propanol, decane,*N*, *N*-dimethylformamide, and thiophene) [22–27]. The experimental procedure consists of four steps [22]: (a) sensor calibration; (b) cell loading; (c) setting up of the experimental conditions; and (d) measurements at equilibrium. In the cell-loading step, the liquid (water, 1-pentanol, or 2-pentanol) is first degassed and then distilled under vacuum, and vigorously stirred in the evacuated cell. Measurements are made at constant temperature; the pressure measurements begin at 1 MPa,

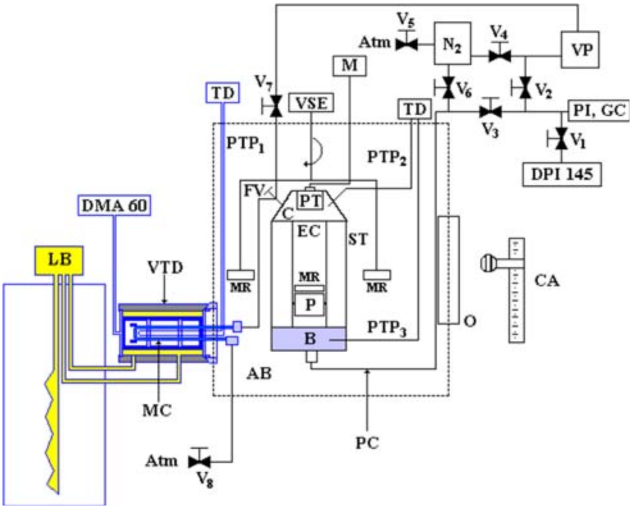

Fig. 1. Schematic flow diagram of the experimental apparatus: AB-air bath; CA-cathetometer; DMA-60 period meter; DPI-145 digital indicator of pressure; EC-sapphire tube equilibrium cell; GC-gas compressor; PI-Isco pump; LB-liquid bath; VTD-vibrating tube densimeter; MC-measurement cell; MR-magnetic rod; PT-pressure transducer; M-multimeter; PTPi−platinum probe i; TD-digital indicator of temperature F250; Vi-shut-off valve i; VSE-variable speed engine; VP-vacuum pump; FV-feeding valve; P-piston; ST-sapphire tube; B-cylindrical support; C-cap; PC-pressurization circuit; O-window.

and then the pressure is increased approximately every 1 MPa up to 25 MPa. Four measurements of the same point are recorded, once the pressure and period signals are kept constant.

2.3.1. Calibration

A detailed procedure of the sensor calibration was given in previous papers [18,22]. A calibration system (Automatic Systems F300S, USA) using a 25-Ω reference probe (Rosemount, England, Model 162CE; ±0.005 K certified uncertainty on the ITS-90 scale) is used to calibrate the three platinum probes. The pressure transducer is calibrated against a deadweight balance (Desgranges & Huot, France, Model 5304; uncertainty ±0.005% full scale). The pressure calibrations are made from 313 to 363 K at the same conditions of the isothermal density determinations. The classic calibration method of the VTD is used to obtain the densities [28]. Periods for water and nitrogen are recorded at the same conditions of the reported data. Reference densities of water and nitrogen are calculated using equations of state reported by Wagner and Pruß [29] and Span et al. [30], respectively. The maximum uncertainties of the density values calculated for water and nitrogen were 0.003% [29] and 0.02% [30], respectively. The uncertainties for the measured variables were estimated to be $T = (\pm 0.03)$ K for temperature, $P = (\pm 0.008)$ MPa for pressure and $\rho = (\pm 0.20)\ \mathrm{kg{\cdot}m^{-3}}$ for density over the complete range of the reported data, as previously published [22,26].

3. RESULTS AND DISCUSSION

In this work, the densities of 1-pentanol were measured from 313.08 to 362.50 K and from 1.002 up to 25.068 MPa. The results (150 points) are listed in Table II. The densities for 2-pentanol were measured from 313.07 to 362.56 K and from 0.997 to 25.023 MPa. The results (150 points) are reported in Table III. For 1-pentanol, compressed liquid densities have been previously reported in the temperature and pressure range reported here; on the other hand, for 2-pentanol only the data reported by Wappmann et al. [15] were found. The data reported here are at different conditions and with lower uncertainty than those reported in Ref. [15] for 2-pentanol. The ranges of temperature and pressure for all available density data from the different sources are listed in Table I.

A 5-parameter, 6-parameter, and 11-parameter BWRS EoS were used to correlate the experimental densities of 1-pentanol and 2-pentanol, and they are described as follows.

The 5-parameter equation [25,26] is expressed by

$$v = \frac{c_1 + c_2 P}{c_3 - \left(c_4/T + c_5\big/T^{1/3}\right) + P} \tag{1}$$

where v is the specific volume.

The 6-parameter equation [27] is expressed by

$$v = \frac{d_1 + d_2 P}{d_3 - d_4 T + d_5 T^{1/2} + d_6 P} \tag{2}$$

The BWRS EoS [1] has 11 parameters and is expressed as follows:

$$\begin{aligned} P = \frac{RT}{V_\mathrm{m}} &+ \frac{\left(B_0 RT - A_0 - C_0\big/T^2 + D_0\big/T^3 - E_0\big/T^4\right)}{V_\mathrm{m}^2} \\ &+ \frac{(bRT - a - d/T)}{V_\mathrm{m}^3} + \frac{\alpha(a + d/T)}{V_\mathrm{m}^6} + \frac{c\left(1 + u\big/V_\mathrm{m}^2\right)\exp\left(-u\big/V_\mathrm{m}^2\right)}{V_\mathrm{m}^3 T^2} \end{aligned} \tag{3}$$

where V_m is the molar volume.

Table II. Compressed Liquid Densities of 1-Pentanol

T(K)	P(MPa)	ρ(kg·m^{-3})	T(K)	P(MPa)	ρ(kg·m^{-3})
313.08	1.015	799.95	323.06	14.011	802.39
313.08	2.006	800.73	323.06	15.006	803.08
313.08	3.004	801.48	323.06	16.012	803.80
313.08	4.027	802.24	323.06	17.001	804.52
313.08	5.014	802.96	323.06	18.017	805.23
313.08	6.009	803.69	323.06	19.016	805.90
313.08	7.031	804.43	323.06	20.031	806.58
313.08	8.026	805.14	323.06	21.016	807.28
313.08	9.032	805.85	323.06	22.004	807.92
313.08	10.018	806.56	323.06	23.022	808.57
313.08	11.024	807.28	323.06	23.992	809.24
313.08	12.018	807.96	323.06	25.028	809.91
313.08	13.032	808.64	332.92	1.002	784.96
313.08	14.019	809.32	332.92	2.010	785.81
313.08	15.011	810.00	332.92	3.007	786.66
313.08	16.016	810.68	332.92	4.024	787.52
313.08	17.025	811.35	332.92	5.011	788.31
313.08	18.016	812.03	332.92	6.011	789.15
313.08	19.016	812.68	332.92	7.012	789.94
313.08	20.028	813.36	332.92	8.017	790.75
313.08	20.996	813.96	332.92	8.985	791.51
313.08	22.031	814.64	332.92	10.018	792.31
313.08	23.018	815.28	332.92	11.006	793.09
313.08	24.026	815.90	332.92	12.013	793.89
313.08	25.031	816.55	332.92	13.010	794.63
323.06	1.019	792.45	332.92	14.014	795.41
323.06	2.009	793.25	332.92	14.984	796.11
323.06	3.006	794.06	332.92	15.982	796.86
323.06	4.036	794.87	332.92	17.027	797.62
323.06	5.025	795.68	332.92	18.029	798.33
323.06	5.964	796.38	332.92	19.006	799.06
323.06	7.031	797.19	332.92	20.000	799.78
323.06	8.015	797.97	332.92	21.011	800.49
323.06	8.986	798.69	332.92	22.015	801.24
323.06	10.003	799.45	332.92	23.008	801.87
323.06	11.017	800.20	332.92	24.015	802.58
323.06	11.986	800.90	332.92	25.044	803.31
323.06	13.011	801.64			
342.82	1.010	777.05	352.67	14.017	780.19
342.82	2.031	777.97	352.67	15.017	780.98
342.82	3.009	778.84	352.67	16.020	781.79

Table II. Continued

T(K)	P(MPa)	ρ(kg·m^{-3})	T(K)	P(MPa)	ρ(kg·m^{-3})
342.82	4.042	779.72	352.67	17.002	782.58
342.82	5.008	780.53	352.67	18.032	783.40
342.82	6.009	781.32	352.67	19.015	784.30
342.82	7.015	782.20	352.67	20.029	785.05
342.82	8.003	783.01	352.67	21.000	785.83
342.82	8.994	783.80	352.67	22.019	786.59
342.82	10.005	784.67	352.67	23.017	787.40
342.82	11.015	785.48	352.67	24.000	788.18
342.82	11.997	786.27	352.67	25.068	788.91
342.82	13.007	787.05	362.50	1.003	759.91
342.82	14.012	787.85	362.50	2.000	760.95
342.82	15.005	788.64	362.50	3.023	762.00
342.82	16.021	789.41	362.50	4.013	762.97
342.82	16.938	790.12	362.50	5.014	763.97
342.82	18.041	790.96	362.50	6.014	764.92
342.82	18.998	791.69	362.50	7.019	765.89
342.82	19.990	792.44	362.50	8.026	766.84
342.82	21.029	793.20	362.50	9.019	767.79
342.82	21.980	793.90	362.50	10.027	768.70
342.82	23.063	794.72	362.50	11.020	769.60
342.82	24.080	795.42	362.50	12.015	770.55
342.82	25.018	796.09	362.50	13.024	771.46
352.67	1.016	768.55	362.50	14.014	772.30
352.67	2.018	769.54	362.50	15.018	773.18
352.67	3.006	770.47	362.50	16.038	774.03
352.67	4.005	771.40	362.50	16.993	774.84
352.67	5.003	772.34	362.50	18.020	775.57
352.67	6.017	773.27	362.50	19.000	776.44
352.67	7.003	774.15	362.50	20.016	777.47
352.67	8.010	775.04	362.50	21.079	778.28
352.67	9.005	775.92	362.50	22.108	779.16
352.67	10.026	776.80	362.50	23.033	779.85
352.67	11.014	777.68	362.50	24.053	780.74
352.67	12.003	778.49	362.50	25.056	781.45
352.67	13.012	779.36			

The Marquardt–Levenberg least-squares optimization was used to correlate the parameters of the models using the following objective function:

$$S=\sum_{i}\left[\left(\rho_i^{\text{exp}}-\rho_i^{\text{cal}}\right)/\rho_{\text{i}}^{\text{exp}}\right]^2 \tag{4}$$

Table III. Compressed Liquid Densities of 2-Pentanol

T(K)	P(MPa)	ρ(kg·m^{-3})	T(K)	P(MPa)	ρ(kg·m^{-3})
313.07	1.006	792.89	323.03	14.034	795.08
313.07	2.014	793.73	323.03	14.992	795.82
313.07	3.011	794.53	323.03	16.006	796.59
313.07	4.037	795.35	323.03	17.011	797.41
313.07	5.027	796.18	323.03	17.997	798.13
313.07	6.022	796.95	323.03	18.996	798.89
313.07	7.038	797.74	323.03	19.992	799.61
313.07	8.056	798.53	323.03	20.993	800.33
313.07	9.036	799.30	323.03	22.010	801.06
313.07	10.019	800.03	323.03	23.001	801.75
313.07	11.022	800.81	323.03	23.980	802.47
313.07	12.024	801.55	323.03	25.023	803.25
313.07	13.014	802.28	332.88	1.023	775.26
313.07	14.016	803.02	332.88	2.008	776.20
313.07	15.002	803.77	332.88	3.002	777.12
313.07	16.018	804.51	332.88	4.018	778.06
313.07	17.004	805.21	332.88	5.000	779.00
313.07	18.021	806.00	332.88	6.006	779.89
313.07	19.016	806.66	332.88	6.985	780.78
313.07	20.027	807.40	332.88	8.007	781.70
313.07	21.004	808.06	332.88	9.008	782.60
313.07	22.032	808.78	332.88	10.011	783.46
313.07	23.012	809.43	332.88	11.003	784.32
313.07	24.018	810.16	332.88	12.011	785.19
313.07	25.021	810.85	332.88	12.989	786.01
323.03	0.997	784.13	332.88	14.011	786.82
323.03	2.021	785.05	332.88	15.005	787.64
323.03	2.999	785.91	332.88	16.011	788.45
323.03	4.039	786.81	332.88	16.985	789.25
323.03	5.019	787.67	332.88	17.995	790.09
323.03	6.013	788.53	332.88	18.995	790.84
323.03	7.016	789.36	332.88	19.996	791.64
323.03	8.004	790.19	332.88	20.990	792.41
323.03	9.023	791.05	332.88	22.000	793.19
323.03	10.009	791.86	332.88	22.983	793.92
323.03	11.011	792.66	332.88	24.027	794.70
323.03	11.998	793.45	332.88	25.001	795.41
323.03	12.995	794.27			
342.77	1.048	765.93	352.63	14.009	769.50
342.77	2.015	766.92	352.63	15.018	770.46
342.77	3.007	767.91	352.63	16.026	771.36
342.77	4.025	768.93	352.63	17.019	772.25
342.77	5.007	769.95	352.63	18.023	773.21
342.77	6.001	770.89	352.63	19.008	774.10
342.77	7.023	771.92	352.63	20.034	775.02

Table III. Continued

T(K)	P(MPa)	ρ(kg·m^{-3})	T(K)	P(MPa)	ρ(kg·m^{-3})
342.77	8.005	772.85	352.63	21.023	775.88
342.77	8.994	773.75	352.63	21.999	776.72
342.77	10.024	774.72	352.63	23.028	777.62
342.77	11.006	775.61	352.63	24.032	778.42
342.77	11.998	776.50	352.63	24.996	779.27
342.77	13.002	777.40	362.56	1.003	745.69
342.77	14.000	778.28	362.56	2.020	746.92
342.77	15.014	779.14	362.56	3.022	748.11
342.77	16.027	780.04	362.56	4.018	749.27
342.77	17.030	780.91	362.56	5.016	750.41
342.77	18.017	781.74	362.56	6.026	751.57
342.77	19.029	782.59	362.56	7.016	752.66
342.77	19.991	783.40	362.56	8.022	753.74
342.77	20.997	784.21	362.56	9.023	754.83
342.77	22.001	785.05	362.56	10.010	755.89
342.77	23.024	785.86	362.56	11.017	756.91
342.77	24.046	786.68	362.56	12.027	757.95
342.77	24.997	787.44	362.56	13.020	758.96
352.63	1.017	756.19	362.56	14.014	759.99
352.63	2.012	757.34	362.56	15.021	760.96
352.63	3.013	758.41	362.56	16.029	761.95
352.63	4.021	759.51	362.56	17.003	762.91
352.63	5.013	760.57	362.56	18.013	763.94
352.63	5.997	761.62	362.56	19.028	764.92
352.63	7.012	762.66	362.56	20.011	765.85
352.63	8.024	763.70	362.56	21.016	766.89
352.63	9.018	764.70	362.56	22.013	767.75
352.63	10.018	765.70	362.56	23.031	768.67
352.63	11.025	766.67	362.56	24.003	769.53
352.63	12.021	767.64	362.56	25.009	770.32
352.63	13.016	768.58			

The statistical values used to evaluate the correlations are the absolute average deviation (AAD), the mean deviation (bias), the standard deviation (SDV), and the root-mean-square deviation (RMS). Expressions for these values were given in previous papers [25–27].

$$\%\Delta V_i = 100\left(\frac{V^{\mathrm{exp}} - V^{\mathrm{cal}}}{V^{\mathrm{exp}}}\right) \tag{5}$$

$$\mathrm{AAD} = \frac{1}{n}\sum_{i=1}^{n} |\%\Delta V_i| \tag{6}$$

$$\mathrm{bias} = \frac{1}{n}\sum_{i=1}^{n} (\%\Delta V_i) \tag{7}$$

$$\mathrm{SDV} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n} (\%\Delta V_i - \mathrm{bias})^2} \tag{8}$$

$$\mathrm{RMS} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (\%\Delta V_i)^2} \tag{9}$$

The parameters for the three equations along with statistical values and the validity range are given in Table IV. The relative deviations of experimental densities reported here (ρ^{exp}) and density values calculated (ρ^{cal}) with Eqs. (1), (2), and (3) are shown in Figs. 2 and 3 for 1-pentanol and 2-pentanol, respectively. From Fig. 2 the maximum relative deviations are ±0.027, ±0.024, and ±0.03, for Eqs. (1), (2), and (3), respectively; and from Fig. 3 the maximum relative deviations are ±0.034, ±0.032, and ±0.038, for Eqs. (1), (2), and (3), respectively. For both liquids the three equations correlated the experimental data within the experimental uncertainty over the range of measurements.

In order to check for the consistency of the experimental densities reported herein, comparisons with published data were performed. Since the conditions of temperature and pressure are different and the correlation models represent the data within the experimental uncertainty, comparisons are made, using relative deviations as defined by Eq. (4), of published and calculated values using the correlations with the adjusted parameters reported in Table IV.

Relative deviations of densities published in the literature (ρ^{lit}) and density values calculated (ρ^{cal}) with Eq. (1) for 1-pentanol are shown in Fig. 4. The validation was performed on points with temperatures and pressures very similar to those of the present work. Good agreement was observed with the data reported by Garg et al. [14] and Zolin et al. [12] and most of the data of Gylmanov et al. [11]. Similar deviations can be obtained using Eq. (2). Extrapolation to higher temperatures and pressures using the BWRS EoS for 1-pentanol are shown in Fig. 5. The equation gave good extrapolations considering that the pressure is 175 MPa and the temperature is 200 K higher than those used to obtain the parameters for the BWRS EoS reported in Table IV. The temperature

Table IV. Parameters for the Correlation Models for 1-Pentanol and 2-Pentanol: Temperature, Pressure, and Density Ranges, Number of Data Points, and Equation Parameters along with Statistical Values

	1-pentanol	**2-pentanol**
T_{min} (K)	313.08	313.07
T_{max} (K)	362.50	362.56
P_{min} (MPa)	1.002	0.997
P_{max} (MPa)	25.068	25.023
ρ_{min} ($\mathrm{kg{\cdot}m^{-3}}$)	759.91	745.69
ρ_{max} ($\mathrm{kg{\cdot}m^{-3}}$)	816.55	810.85
n	150	150
5-parameters		
c_1($\mathrm{MPa{\cdot}kg^{-1}{\cdot}m^3}$)	0.18756	0.15782
c_2($\mathrm{kg^{-1}{\cdot}m^3}$)	1.066×10^{-3}	1.088×10^{-3}
c_3(MPa)	−422.60	−448.47
c_4(K·MPa)	69904.6	70350.1
c_5 ($\mathrm{MPa{\cdot}K^{1/3}}$)	−5403.4	−5419.5
AAD (%)	0.008	0.013
bias (%)	0.003	0.006
SDV (%)	0.009	0.015
RMS (%)	0.01	0.02
6-parameters		
d_1 ($\mathrm{MPa{\cdot}m^3{\cdot}kg^{-1}}$)	−10.6752	−3.6023
d_2 ($\mathrm{m^3{\cdot}kg^{-1}}$)	−0.06065	−0.02483
d_3 (MPa)	−3257.0	−639.6
d_4 ($\mathrm{MPa{\cdot}K^{-1}}$)	−32.342	−13.190
d_5 ($\mathrm{MPa{\cdot}K^{-1/2}}$)	−870.33	−358.44
d_6	−56.92	−22.83
AAD (%)	0.007	0.010
bias (%)	0.001	−0.002
SDV (%)	0.009	0.012
RMS (%)	0.01	0.01
BWRS EoS		
B_0 ($\mathrm{cm^3{\cdot}mol^{-1}}$)	435.22	681.10
A_0 ($\mathrm{bar{\cdot}cm^6{\cdot}mol^{-2}}$)	3.3515×10^7	3.4689×10^7
C_0 ($\mathrm{bar{\cdot}K^2{\cdot}cm^6{\cdot}mol^{-2}}$)	8.3525×10^{11}	5.0313×10^{11}
D_0 ($\mathrm{bar{\cdot}K^3{\cdot}cm^6{\cdot}mol^{-2}}$)	-2.0026×10^{14}	-1.7480×10^{14}
E_0 ($\mathrm{bar{\cdot}K^4{\cdot}cm^6{\cdot}mol^{-2}}$)	-1.2313×10^{17}	-1.0927×10^{17}
b ($\mathrm{cm^6{\cdot}mol^{-2}}$)	3.6032×10^4	1.6939×10^4
a ($\mathrm{bar{\cdot}cm^9{\cdot}mol^{-3}}$)	1.8759×10^8	1.6714×10^8
d ($\mathrm{bar{\cdot}K{\cdot}cm^9{\cdot}mol^{-3}}$)	1.7473×10^{10}	2.9958×10^{10}
c ($\mathrm{bar{\cdot}K^2{\cdot}cm^9{\cdot}mol^{-3}}$)	-2.3547×10^{14}	-2.6375×10^{14}
α ($\mathrm{cm^9{\cdot}mol^{-3}}$)	2.0022×10^7	2.0089×10^7
u ($\mathrm{cm^6{\cdot}mol^{-2}}$)	9.6228×10^3	5.3111×10^3
AAD (%)	0.007	0.010
bias (%)	−0.0001	−0.001
SDV (%)	0.009	0.012
RMS (%)	0.01	0.01

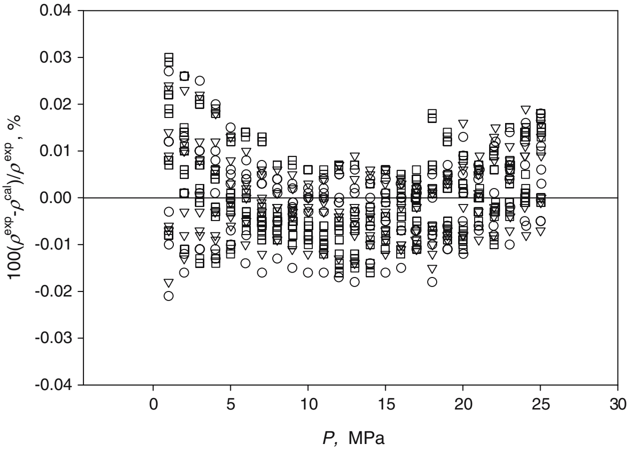

Fig. 2. Relative deviations of experimental densities from this work (ρ^{exp}) and values calculated (ρ^{cal}) with three different equations using the parameters reported in Table IV for 1-pentanol; ○, Eq. (1); ▽, Eq. (2), □, BWRS EoS.

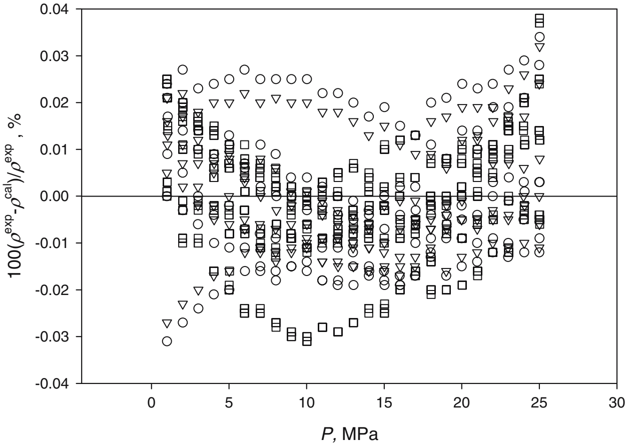

Fig. 3. Relative deviations of experimental densities from this work (ρ^{exp}) and values calculated (ρ^{cal}) with three different equations using the parameters reported in Table IV for 2-pentanol; ○, Eq. (1); ▽, Eq. (2), □, BWRS EoS.

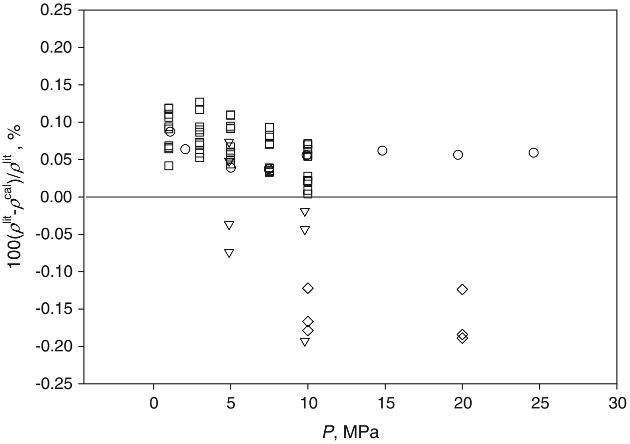

Fig. 4. Relative deviations of experimental densities from literature results (ρ^{lit}) and values calculated (ρ^{cal}) with Eq. (1) using the parameters reported in Table IV for 1-pentanol; ▽, Gylmanov et al. [11]; ○, Zolin et al. [12]; □, Garg et al. [14]; ◇, Wappmann et al. [15].

extrapolation plotted in Fig. 5 is up to 549.42 K; perhaps, at higher temperatures deviations with literature data [12] and calculated values increase strongly. These results are not plotted in Fig. 5.

Comparisons of densities calculated with the three equations with data reported by Wappmann et al. [15] for 2-pentanol are shown in Fig. 6. Data from 80 to 200 MPa at 342.9 K reported by Wappmann et al. [15] for 2-pentanol are probably erroneous. The three equations were in good agreement with the data reported by Wappmann [15], over the ranges of temperature and pressure measured here as can be seen in Fig. 6, where the two black lines at 10 and 20 MPa represent the relative deviations between literature data and values calculated with the three equations. The maximum relative deviations observed were ±0.15%. These results are in agreement within the experimental uncertainty of ±0.4% in the pressure range up to 100 MPa reported in Ref. [15]. Relative deviations of experimental data from literature values at atmospheric pressure [14,31–37] and density values calculated with Eq. (1) for 1-pentanol and 2-pentanol are shown in Figs. 7 and 8, respectively. Good extrapolations were obtained for the temperature range employed here. The deviation increased as the temperature decreased. Similar results were obtained for Eq. (2) and the BWRS EoS for both liquids; for convenience, only the results for Eq. (1) were plotted.

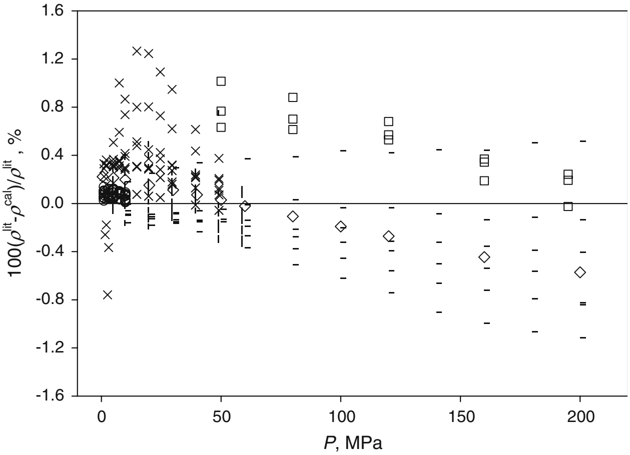

Fig. 5. Relative deviations of experimental densities from literature results (ρ^{lit}) and values calculated (ρ^{cal}) with the BWRS EoS using the parameters reported in Table IV for 1-pentanol; |, Gylmanov et al. [11]; ×, Zolin et al. [12]; ◇, Altunin and Konikevich [13]; ○, Garg et al. [14]; –, Wappmann et al. [15]. □, Sülzner et al. [16].

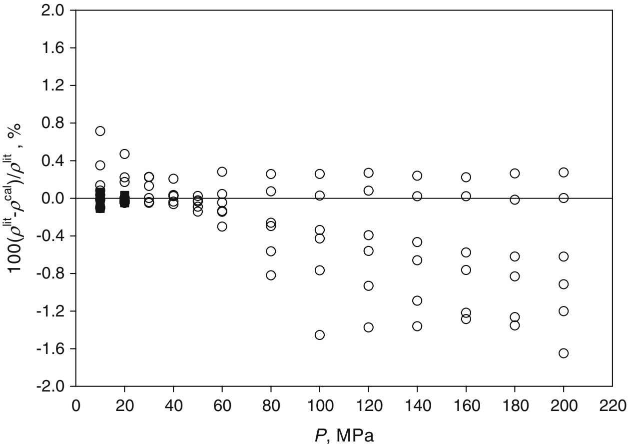

Fig. 6. Relative deviations between experimental densities from Wappmann et al. [15] and density values calculated with the three equations used in this work; ●, Eq. (1); ■, Eq. (2); ○, BWRS EoS.

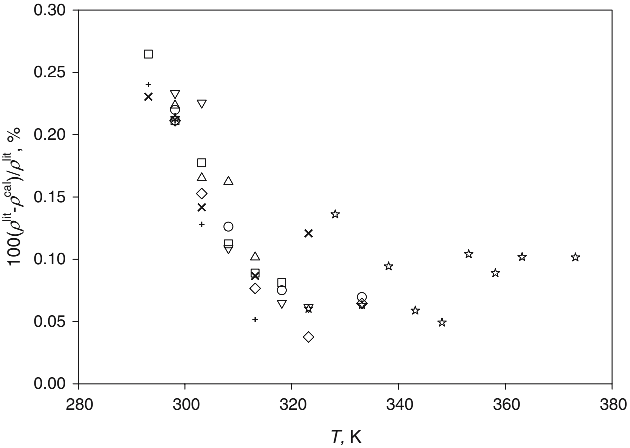

Fig. 7. Relative deviations of experimental densities from literature (ρ^{lit}) and values calculated (ρ^{cal}) with Eq. (1) for 1-pentanol at atmospheric pressure; ○, Diaz-Peña and Tardajos [31]; □, Ortega and Paz-Andrade [32]; △, Riggio et al. [33]; ◇, Ortega [34]; ▽, Garcia et al. [35]; ☆, Garg et al. [14]; ×, Indraswati et al. [36]; +, Rodriguez et al. [37].

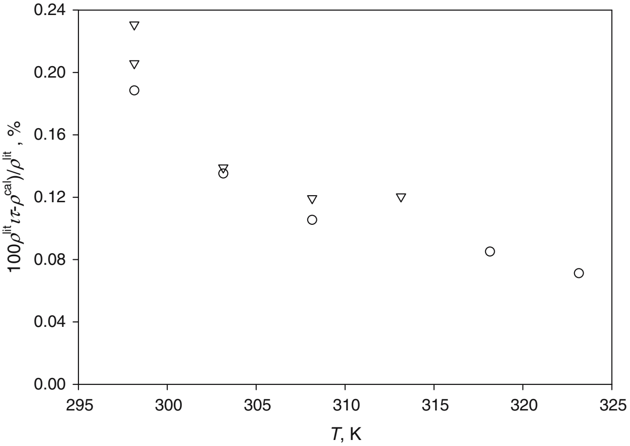

Fig. 8. Relative deviations of experimental densities from literature (ρ^{lit}) and values calculated (ρ^{cal}) with Eq. (1) for 2-pentanol at atmospheric pressure, data from: ○, Ortega [32]; ▽, Riggio et al. [33].

4. CONCLUSIONS

Reliable compressed liquid densities of 1-pentanol and 2-pentanol were measured with the help of a vibrating tube densimeter. The experimental data can be described within experimental uncertainty by the three equations used in this work; however, extrapolation to higher pressures and temperatures using the two short equations was not reliable. For this case, the BWRS EoS gave deviations of less than ±1.3% for 1-pentanol at temperatures up to 549.42 K and at pressures up to 200 MPa; and for 2-pentanol the maximum relative deviations were less than ±1.7% at temperatures up to 433 K and at pressures up to 200 MPa. The eleven parameters of the BWRS EoS allow reliable extrapolations at high temperature and pressure.

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