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Densities of 1-Propanol and 2-Propanol via a Vibrating Tube Densimeter from 313 to 363 K and up to 25 MPa

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PvT properties were determined in the liquid phase for 1-propanol and 2-propanol from 313 to 363 K and up to 25 MPa with an uncertainty lower than ±0.05%. The calibration method of the vibrating tube densimeter was performed with N_2 and H_2O as reference fluids. The 1-propanol and 2-propanol liquid densities reported in this work are correlated with an eleven-parameter equation of state of Starling and Han (BWRS) and the Tait equation using a least-squares optimization, with a relative deviation lower than ±0.05% for both fluids. The density values calculated by the BWRS equation of state and the Tait equation agree within 0.05% with data reported by Yaginuma et al.[15] for 1-propanol and within 0.09% with data reported by Yaginuma et al.[16] for 2-propanol.

Introduction

PvT properties of pure compounds, *PvT* properties and phase equilibria (vapor−liquid, vapor−liquid−liquid, and liquid−liquid equilibria), and mixtures at high pressures are required in the development of supercritical fluid extraction processes. Supercritical fluids containing CO_2 and alcohols are interesting from both theoretical and practical points of view, especially for the processing of pharmaceutical and natural products.[1,2]

Our research is focused on a systematic study to obtain experimental VLE and *PvT* data of the CO_2−alcohol mixtures for knowledge, development, and application of techniques directed toward supercritical extraction processes. The main objective is to perform systematic studies of *PvT* and phase equilibria[3−11] of binary mixtures containing CO_2 and alcohol (from ethanol to decanol) in order to select the best supercritical operating conditions required for industrial applications, such as extraction of carotenes from the chili Poblano of Mexico (*Capsicum annum*).

Compressed liquid densities, for 1-propanol and 2-propanol, from 313 to 363 K and from 0.5 MPa to 25 MPa, are reported here. The reliability of the measurements has been checked by comparing the data calculated through the Starling and Han equation of state (BRWS EoS) and the Tait equation fitted on data reported in this work and data from other authors.

Experimental Section

Apparatus and Procedure. A detailed description of the apparatus used in this work has been given by Zuñiga-Moreno and Galicia-Luna.[3] The measuring cell (see Figure 1) is composed of a vibrating tube (Hastelloy C-276 U-tube) with a 1 cm^3 internal volume. The experimental procedure used here is that already described by Galicia-Luna et al.[4] and Zuñiga-Moreno and Galicia-Luna.[3] In this work, estimated uncertainties are ±0.03 K for temperatures, ±0.008 MPa for pressures, and ±0.05% for liquid densities.

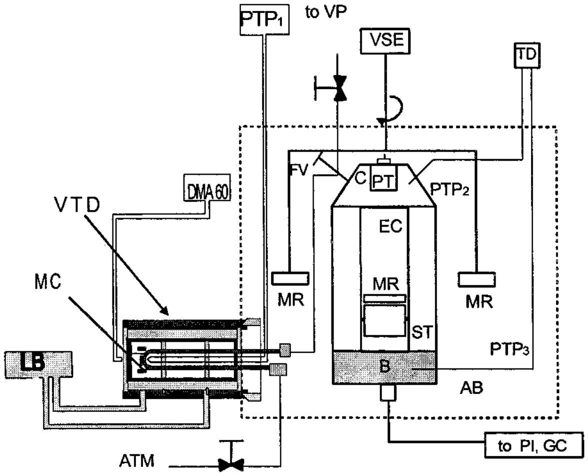

Figure 1. Simplified flow diagram of the apparatus: AB, air bath; B and C, caps in titanium; DMA 60, period meter; EC, equilibrium cell; FV, feeding valve; GC, gas compressor; LB, liquid bath; MC, measurement cell; MR, magnetic rod; PI, Isco pump; PT, pressure transducer; PTP*i*, platinum probe *i*; ST, sapphire tube; TD, digital indicator of temperature F250; VSE, variable speed engine; VP, vacuum pump; VTD, vibrating tube densimeter.

The experimental procedure consists of four steps: 1, sensor calibration; 2, cell loading; 3, setting up of the experimental conditions; and 4, measurements at equilibrium. A detailed calibration procedure of the platinum temperature probes and of the pressure transducer is given elsewhere by Galicia-Luna et al.[3,5]

The platinum probes Pt 100 (PTP_1, PTP_2, and PTP_3, Specitec, France; see Figure 1) connected to a digital indicator (Automatic Systems F250, USA) were calibrated against a calibration system (Automatic Systems F300S, USA) connected to a 25-Ω reference probe (model 162CE of ±0.005 K certified accuracy on the ITS-90 scale, from Rosemount, England).

The Sedeme (25 MPa, France) pressure transducer connected to a 6 $^1/_2$ digital multimeter (HP-34401A, USA) is calibrated at temperatures from 313 to 363 K against a dead weight balance (Desgranges & Huot, France, Model

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Table 1. Purity and Origin of Pure Compounds

compound	certified purity (%)	max. water content (%)	supplier
1-propanol	99.5	0.05	Merck
2-propanol	99.5	0.05	Merck
CO_2	99.995		Air Products-Infra
water	99.95 (HPLC)		Fisher
nitrogen	99.995		Air Products-Infra

Table 2. Densities of Pure Liquids and Comparison with Literature[17] Values at Different Temperatures

	ρ/kg·m^{-3}			
	1-propanol		2-propanol	
T/K	exptl[a]		exptl[a]	
298.07	799.33		781.07	
303.26	795.45		776.69	
313.23	788.08		768.69	
321.74	779.32		761.10	
	cal[b]	lit.[17]	cal[c]	lit.[17]
298.15	799.20	799.58	780.92	781.23
303.15	795.99	795.48	776.94	776.95
308.15	792.24	791.38	772.84	772.46
313.15	787.96	787.37	768.63	767.98

[a] Experimental data in this work. [b] Equation for 1-propanol: $\rho_1 = -(1.069086 \times 10^{-02})T^2 + 5.785885T + 24.48764$. Standard deviation/kg·m^{-3} = 0.222. [c] Equation for 2-propanol: $\rho_2 = -(2.272116 \times 10^{-03})T^2 + (5.69641 \times 10^{-01})T + 813.0550$. Standard deviation/kg·m^{-3} = 0.223.

5304; accuracy ±0.005% full scale). The calibration was done by both increasing and decreasing the pressure at a constant temperature to check for hysteresis.

The vibrating tube was calibrated using water and nitrogen. The reference density values for the H_2O and N_2 compounds were computed using the equations of state (EoS) of Harr et al.[12] and Span et al.[13]

The density of the fluid inside the U-tube, ρ_F, is given by

$$\rho_F(P,T) = \rho_{H_2O}(P,T) + \frac{1}{A}(P,T)(\tau_F^2(P,T) - \tau_{H_2O}^2(P,T)) \quad (1)$$

where $\rho_F(P,T)$ and $\tau_F^2(P,T)$ are the density and vibration period, respectively, of 1-propanol or 2-propanol and

$$\frac{1}{A} = \frac{\rho_{H_2O} - \rho_{N_2}}{\tau_{H_2O}^2 - \tau_{N_2}^2} \quad (2)$$

The purity and origin of chemicals used in this work are given in Table 1. The purities of the liquid samples were tested using a gas chromatograph (HP 5890 Series II) fitted with a flame ionization detector and a packed column. The verified guaranteed purities are in both cases >99.5%. Alcohols were stored over 3A molecular sieves to avoid any moisture and were used without any further purification except for a careful degassing.

Theory. The experimental data have been correlated using the Starling and Han equation of state (BWRS EoS):[14]

$$P = \frac{RT}{v} + \left(B_0RT - A_0 - \frac{C_0}{T^2} + \frac{D_0}{T^3} - \frac{E_0}{T^4}\right)/v^2 + (bRT - a - d)/v^3 + \alpha\left(a + \frac{d}{T}\right)/v^6 + c\left(1 + \frac{u}{v^2}\right)\exp\left(-\frac{u}{v^2}\right)/(v^3T^2) \quad (3)$$

where v is the molar volume.

And using the Tait equation[15]

$$\rho = \rho_0/\left[1 - C\ln\left(\frac{B_T + P}{B_T + P_0}\right)\right] \quad (4)$$

Both equations are useful for the description of compressed liquid densities.

Table 3. Densities of 1-Propanol at Different Temperatures

T/K = 313.15		T/K = 323.10		T/K = 332.99		T/K = 342.95		T/K = 352.88		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}
0.500	788.29	0.511	779.97	0.507	771.54	0.511	762.53	0.509	753.47	0.513	743.92
1.005	788.71	1.022	780.44	1.005	772.03	1.008	763.04	1.026	754.05	1.013	744.53
2.010	789.57	2.009	781.33	2.015	772.99	2.008	764.07	2.014	755.14	2.016	745.73
3.033	790.45	3.014	782.25	3.005	773.96	3.012	765.09	3.001	756.22	3.010	746.90
4.002	791.26	4.014	783.14	4.016	774.90	4.024	766.12	3.998	757.30	4.006	748.06
5.007	792.10	5.002	784.02	5.017	775.85	5.031	767.12	5.004	758.39	5.010	749.20
6.006	792.93	6.025	784.91	6.027	776.79	6.007	768.10	6.005	759.44	6.010	750.33
7.004	793.76	7.013	785.77	7.024	777.72	7.018	769.08	7.015	760.48	7.015	751.46
8.010	794.58	8.016	786.66	8.010	778.61	8.011	770.05	8.003	761.51	8.007	752.55
8.998	795.39	9.023	787.52	9.016	779.52	9.015	771.02	9.030	762.56	9.013	753.64
10.006	796.20	9.998	788.35	10.028	780.42	10.007	771.95	10.001	763.53	10.003	754.71
11.004	796.99	11.041	789.22	11.010	781.29	11.008	772.88	11.019	764.54	10.999	755.76
12.004	797.78	12.002	790.02	12.027	782.17	12.025	773.82	12.002	765.50	12.019	756.81
12.997	798.57	13.017	790.85	12.999	783.01	13.013	774.72	13.021	766.49	12.988	757.82
14.008	799.34	14.007	791.65	14.050	783.90	14.016	775.61	13.997	767.42	14.016	758.84
14.990	800.08	15.002	792.45	15.017	784.72	14.992	776.49	15.016	768.38	15.006	759.84
16.024	800.85	16.011	793.24	15.994	785.53	16.028	777.39	16.004	769.29	16.008	760.82
16.994	801.58	17.038	794.04	17.030	786.38	17.000	778.24	16.997	770.21	17.026	761.81
18.005	802.32	17.999	794.80	18.005	787.17	18.029	779.12	18.027	771.14	18.006	762.75
19.000	803.05	19.023	795.57	19.021	787.99	19.013	779.95	19.009	772.02	19.009	763.71
20.019	803.79	20.036	796.33	20.006	788.78	20.002	780.78	20.026	772.94	20.031	764.66
20.986	804.49	21.002	797.08	21.026	789.59	21.034	781.64	21.002	773.79	21.045	765.61
22.024	805.23	22.016	797.82	22.018	790.38	22.046	782.48	22.006	774.67	21.992	766.49
22.993	805.93	23.037	798.60	23.024	791.17	23.000	783.28	23.082	775.60	23.029	767.45
24.040	806.70	23.994	799.34	24.007	791.95	24.036	784.14	24.059	776.45	24.020	768.34
25.003	807.40	25.049	800.13	25.015	792.76	25.090	784.99	25.032	777.29	25.007	769.24
14.006[1]	799.29										
5.008[1]	792.02										
1.008[1]	788.67										
0.499[1]	788.23										

[a] Measurement of densities on decreasing the pressure after its increment up to 25 MPa.

Table 4. Densities of 2-Propanol at Different Temperatures

T/K = 313.16		T/K = 323.11		T/K = 333.02		T/K = 342.97		T/K = 352.93		T/K = 362.81	
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}
0.498	769.30	0.510	760.23	0.498	751.84	0.509	741.69	0.523	731.18	0.507	719.60
1.011	769.80	1.003	760.73	1.006	752.40	1.004	742.30	1.011	731.83	1.011	720.34
2.008	770.76	2.014	761.78	2.008	753.53	2.016	743.51	2.008	733.15	2.013	721.78
3.013	771.70	2.999	762.80	3.010	754.62	3.006	744.68	3.016	734.45	3.003	723.19
4.004	772.64	4.015	763.81	3.995	755.68	4.013	745.87	4.004	735.70	4.008	724.58
5.007	773.59	5.008	764.82	5.018	756.79	5.017	747.04	5.007	736.96	5.005	725.95
6.009	774.52	6.003	765.80	6.008	757.84	6.012	748.18	6.016	738.20	6.012	727.30
7.016	775.44	7.007	766.80	7.009	758.89	7.009	749.30	7.005	739.42	7.010	728.62
8.011	776.36	8.014	767.77	8.026	759.93	8.021	750.42	8.014	740.63	8.004	729.92
9.024	777.27	9.019	768.74	9.004	760.94	9.013	751.50	9.010	741.80	9.018	731.21
10.025	778.16	10.003	769.67	10.013	761.95	10.029	752.60	10.007	742.96	10.011	732.46
11.000	779.02	11.052	770.64	11.016	762.94	11.027	753.66	11.022	744.11	10.997	733.66
12.017	779.90	12.005	771.54	12.003	763.91	12.003	754.68	11.997	745.22	12.013	734.90
13.015	780.76	13.021	772.44	13.023	764.89	13.026	755.73	13.004	746.33	12.993	736.07
13.999	781.58	14.000	773.33	14.003	765.83	14.052	756.77	14.018	747.43	14.024	737.27
15.016	782.44	15.033	774.23	15.025	766.77	15.005	757.72	15.011	748.49	14.997	738.38
16.003	783.26	16.000	775.07	16.000	767.69	16.028	758.74	16.029	749.56	16.021	739.55
17.006	784.06	17.011	775.95	17.026	768.61	16.998	759.68	16.998	750.56	17.001	740.66
18.001	784.86	18.023	776.80	17.997	769.50	18.025	760.67	18.026	751.64	18.031	741.78
19.019	785.67	18.994	777.63	19.038	770.43	19.003	761.60	18.999	752.62	19.013	742.85
20.000	786.45	20.037	778.48	19.994	771.27	19.993	762.54	20.029	753.64	19.998	743.92
21.030	787.25	21.000	779.30	21.003	772.14	21.021	763.49	20.991	754.60	21.023	744.99
21.997	788.01	22.019	780.13	22.048	773.06	21.999	764.40	22.028	755.63	21.996	746.00
23.050	788.83	23.036	780.97	22.999	773.89	23.033	765.34	22.999	756.57	23.020	747.07
24.003	789.60	23.995	781.77	24.025	774.78	23.998	766.23	24.038	757.58	24.020	748.10
25.005	790.39	25.036	782.62	25.118	775.71	25.046	767.18	25.020	758.52	24.998	749.12

Table 5. Tait and Rackett Equations: Adjusted Parameters for 1-Propanol and 2-Propanol

range	1-propanol	2-propanol
T_{min}/K	313.15	313.16
T_{max}/K	362.77	362.80
P_{min}/MPa	0.500	0.498
P_{max}/MPa	25.090	25.118
ρ_{min}/kg·m^{-3}	743.92	719.60
ρ_{max}/kg·m^{-3}	807.40	790.39
no. data points	160	156

Tait parameters	1-propanol	2-propanol
C	0.087 295 461	0.083 655 791
B_0	234.9514	217.713 34
b_1	−50.274 305	−49.319 841
E	100	100
STD/kg·m^{-3}	7.24×10^{-2}	2.22×10^{-1}
P_{ref}/MPa	0.1	0.1

Rackett parameters[a]	1-propanol	2-propanol
A_R	0.082 166 243	0.162 350 64
B_R	0.290 087 31	0.418 726 76
C_R	507.261 76	428.781 87
D_R	0.198 252 05	0.183 616 64

[a] Parameters to calculate densities are in g·cm^{-3}.

Table 6. BWRS EoS Adjusted Parameters[a] for 1-Propanol and 2-Propanol

parameter[1]	1-propanol	2-propanol
B_0	$1.982\,933\,2 \times 10^{2}$	$3.655\,364\,6 \times 10^{2}$
A_0	$1.751\,420\,1 \times 10^{7}$	$2.006\,651\,8 \times 10^{7}$
C_0	$-2.608\,175\,1 \times 10^{11}$	$-4.041\,684\,1 \times 10^{11}$
D_0	$-3.896\,452\,1 \times 10^{14}$	$-2.504\,713\,5 \times 10^{14}$
E_0	$-6.655\,865\,0 \times 10^{16}$	$-7.975\,766\,1 \times 10^{16}$
b	$1.249\,195\,1 \times 10^{4}$	$7.520\,386\,2 \times 10^{3}$
a	$3.296\,645\,2 \times 10^{7}$	$3.700\,938\,9 \times 10^{7}$
d	$3.244\,628\,4 \times 10^{9}$	$6.116\,896\,6 \times 10^{9}$
c	$-6.088\,467\,0 \times 10^{13}$	$-9.962\,965\,3 \times 10^{13}$
α	$9.134\,493\,5 \times 10^{6}$	$9.428\,701\,2 \times 10^{6}$
u	$1.612\,247\,0 \times 10^{4}$	$3.091\,514\,6 \times 10^{3}$
STD/cm^3·mol^{-1}	1.02×10^{-2}	2.63×10^{-1}

[a] The units used for the adjustment of parameters are bar, K, and cm^3·mol^{-1}.

Table 7. Densities of Pure Components from the Literature[16] and Comparison with Calculated Values from the BWRS EoS

	ρ/kg·m^{-3}			
T/K	1-propanol		2-propanol	
	lit.[16]	BWRS	lit.[16]	BWRS
298.15	799.58	799.93	781.23	779.83
303.15	795.48	796.07	776.95	776.40
308.15	791.38	792.11	772.46	772.73
313.15	787.37	788.07	767.98	768.83

We have used the Marquardt−Levenberg least squares optimization using the following objective function, S:

$$S = \sum_i \left[\frac{(\rho_{i,\mathrm{exp}} - \rho_{i,\mathrm{cal}})}{\rho_{i,\mathrm{exp}}}\right]^2 \tag{5}$$

to correlate the parameters of both models. The units used for the adjustment of parameters are bar, kelvin, and cubic centimeters per mole.

For 1-propanol and 2-propanol a reference pressure $P_0 = 0.1$ MPa was chosen. The corresponding liquid densities at atmospheric pressure can be described with a modified Rackett equation,[15]

$$\rho_0 = A_R/B_R^{[1+(1-T/C_R)^{D_R}]} \tag{6}$$

The parameters for this equation were extrapolated from high-pressure experiments. Prof. Gmehling's group provided the correlated parameters[15] reported in Table 5 for 1-propanol and 2-propanol. To consider the temperature dependence in the Tait equation, the following function is used:

$$B_T = b_0 + b_1\frac{T}{E} + b_2\left(\frac{T}{E}\right)^2 + b_3\left(\frac{T}{E}\right)^3 + b_4\left(\frac{T}{E}\right)^4 \tag{7}$$

In the process to correlate the compressed liquid densities for both fluids, eq 7 was used, but it was found that similar results were obtained only retaining his linear terms. This approach is described in detail by Ihmels and Gmehling.[15]

Table 8. Comparison of Calculated Values Using the BWRS EoS and the Tait Equation with Literature[19] Density Values of 1-Propanol at 298.15 K

P/MPa	$\rho^{\mathrm{lit.19}}$/kg·m^{-3}	ρ^{BWRS}/kg·m^{-3}	$((\rho^{\mathrm{lit.18}} - \rho^{\mathrm{BWRS}})/\rho^{\mathrm{lit.18}}) \times 100$	ρ^{Tait}/kg·m^{-3}	$((\rho^{\mathrm{lit.18}} - \rho^{\mathrm{Tait}})/\rho^{\mathrm{lit.18}}) \times 100$
2.00	801.00	801.38	−0.047	801.45	−0.057
5.99	803.90	804.38	−0.060	804.61	−0.088
7.98	805.30	805.85	−0.068	806.14	−0.104
11.97	808.10	808.74	−0.079	809.13	−0.127
15.96	810.90	811.57	−0.083	812.02	−0.138
19.95	813.50	814.34	−0.104	814.81	−0.161
23.93	816.10	817.04	−0.116	817.52	−0.174
28.92	819.30	820.37	−0.130	820.80	−0.183
33.90	822.40	823.59	−0.145	823.95	−0.189

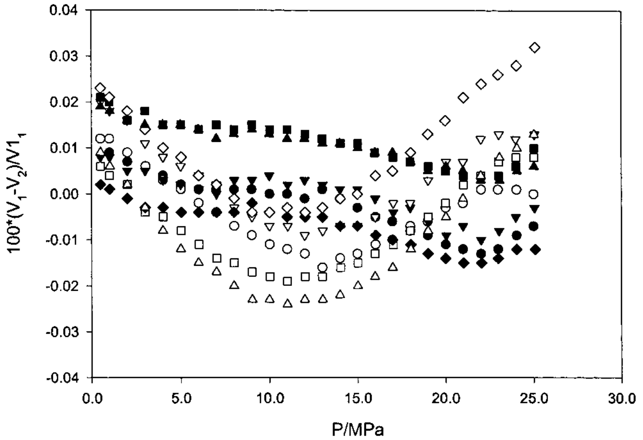

Figure 2. Relative deviations between experimental data (V_1) and those calculated with the BWRS EoS and the Tait equation (V_2) fitted on data reported in this work for 1-propanol at the following temperatures: ●, 313.15 K; ▼, 323.10 K; ■, 332.99 K; ▲, 352.88 K; ◆, 362.77 K. Open and closed symbols are for Tait and BRWS equations, respectively.

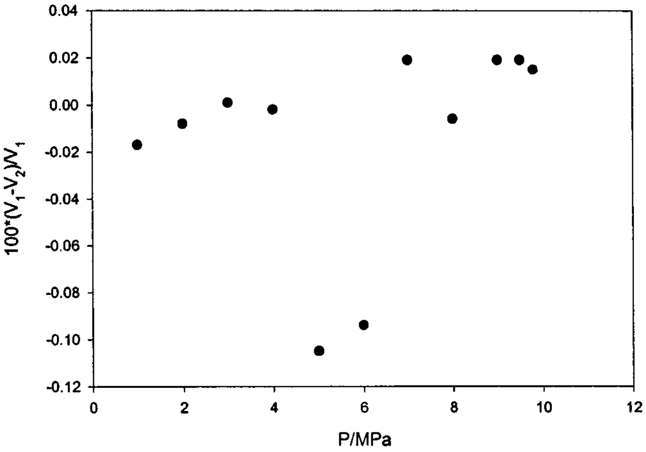

Figure 3. Comparison of the experimental molar volumes from ref 17 (V_1) for 1-propanol with the values calculated with the BWRS EoS (V_2) fitted on data reported in this work at 313.15 K.

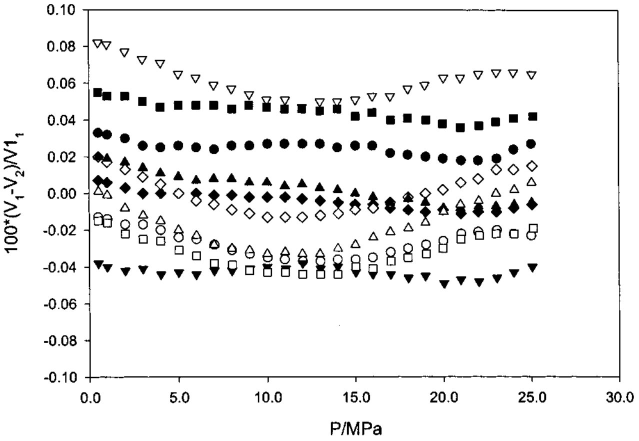

Figure 4. Relative deviations between experimental data (V_1) and those calculated with the BWRS EoS and the Tait equation (V_2) fitted on data reported in this work for 2-propanol at the following temperatures: ●, 313.15 K; ▼, 323.10 K; ■, 332.99 K; ▲, 352.93 K; ◆, 362.77 K. Open and closed symbols are for Tait and BRWS equations, respectively.

Table 9. Comparison of Calculated Data at 313.15 K with the BWRS EoS for 1-Propanol with Data from ref 17

P/MPa	ρ^{BWRS}/kg·m^{-3}	ρ^{exp}/kg·m^{-3}	$((\rho^{\mathrm{exp}} - \rho^{\mathrm{BWRS}})/\rho^{\mathrm{exp}}) \times 100$
1.000	788.73	788.60	−0.017
2.000	789.56	789.50	−0.008
3.000	790.39	790.40	0.001
4.000	791.22	791.20	−0.002
5.000	792.03	791.20	−0.105
6.000	792.84	792.10	−0.094
7.000	793.65	793.80	0.019
8.000	794.45	794.40	−0.006
9.000	795.25	795.40	0.019
9.500	795.65	795.80	0.019
9.800	795.88	796.00	0.015

Results

The densities of pure liquids reported in Table 2 and the corresponding data calculated through both correlations for both fluids were compared with the experimental data of Nikam et al.[16]

The obtained results at atmospheric pressure agree within ±0.86 kg·m^{-3} for 1-propanol and ±0.65 kg·m^{-3} for 2-propanol (se Table 2) with those reported by Nikam et al.[16]

The liquid densities of 1-propanol and 2-propanol were determined at six temperatures from 313 to 363 K (see Tables 3 and 4) and compared with the data of Yaginuma et al.[17,18] For the comparison, the data reported in this work were correlated for the whole range of pressures and temperatures reported using the BWRS EoS[14] and the Tait equation. The obtained parameters for the different equations and their standard deviations (STDs) are given in Tables 5 and 6. Relative deviations between experimental data (V_1 experimental molar volume) and those calculated with the BWRS EoS and the Tait equation (V_2 calculated molar volume) fitted to the data reported in this work for 1-propanol and 2-propanol are presented in Figures 2 and 4. The maximum relative deviations $100(V_1 - V_2)/V_1$ from Figure 2 are +0.032% and −0.125% for 1-propanol, and from Figure 4 are +0.082% and −0.05% for 2-propanol, and the standard deviations (STDs) are given in Tables 5 and 6.

The calculated values for 1-propanol and 2-propanol using the BRWS EoS were compared with those published by Nikam et al.[16] at atmospheric pressure liquid densities, and both of them agree (see Table 7).

The densities of 1-propanol and 2-propanol correlated to the BWRS EoS[14] were compared with the experimental

Table 10. Comparison of Calculated Values Using the BWRS EoS and the Tait Equation with Literature^{20} Density Values of 2-Propanol at Different Temperatures

T/K	P/MPa	$\rho^{\mathrm{lit.19}}$/kg·m^{-3}	ρ^{BWRS}/kg·m^{-3}	$((\rho^{\mathrm{lit.19}} - \rho^{\mathrm{BWRS}})/\rho^{\mathrm{lit.19}}) \times 100$	ρ^{Tait}/kg·m^{-3}	$((\rho^{\mathrm{lit.19}} - \rho^{\mathrm{Tait}})/\rho^{\mathrm{lit.19}}) \times 100$
303.15	0.1	776.40	776.40	0.00		
303.15	20.0	793.00	792.89	0.01	793.45	−0.06
303.15	40.0	806.70	807.20	−0.06	807.29	−0.07
303.15	60.0	818.40	819.87	−0.18	819.16	−0.09

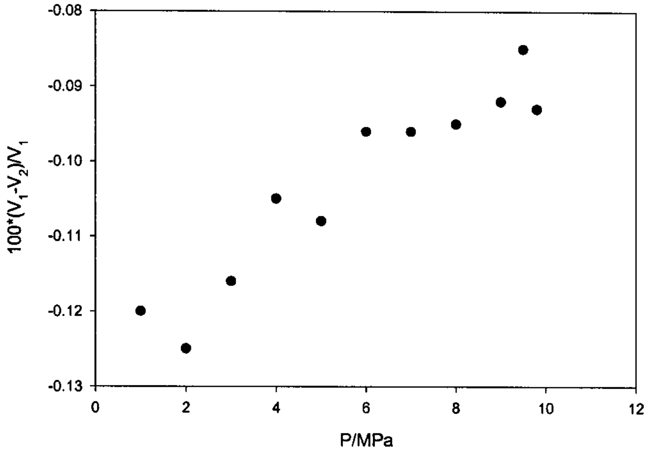

Figure 5. Percent relative deviation calculations between the experimental data of Yaginuma et al.[18] (V_1) for 2-propanol and the values of the BWRS EoS (V_2) fitted on data reported in this work at 313.15 K.

Table 11. Comparison of Calculated Data at 313.15 K with the BWRS EoS for 2-Propanol with Experimental Data from ref 18

P/MPa	ρ^{BWRS}/kg·m^{-3}	ρ^{exp}/kg·m^{-3}	$((\rho^{\mathrm{exp}} - \rho^{\mathrm{BWRS}})/\rho^{\mathrm{exp}}) \times 100$
1.000	769.62	768.7	−0.120
2.000	770.56	769.6	−0.125
3.000	771.49	770.6	−0.116
4.000	772.41	771.6	−0.105
5.000	773.34	772.5	−0.108
6.000	774.24	773.5	−0.096
7.000	775.14	774.4	−0.096
8.000	776.03	775.3	−0.095
9.000	776.92	776.2	−0.092
9.500	777.36	776.7	−0.085
9.800	777.62	776.9	−0.093

values of data reported by Yaginuma et al.[17−18] The obtained results agree quite well with those of Yaginuma et al.[17] (see Figure 3 and Table 9) and Yaginuma et al.[18] (see Figure 5 and Table 11). The maximum relative deviations from Figure 3 are +0.02% and −0.11%, and that from Figure 5 is −0.125%.

To demonstrate the versatility of the models used in this study, the densities were calculated outside the range of parameters adjustment. In doing so, it was noted that the models provide excellent results, as can be observed by examining results given in Table 8 of ref 19 for 1-propanol and Table 10 of ref 20 for 2-propanol.

The temperatures were selected taking into account the intended industrial applications of CO_2 and of binary mixtures containing CO_2 and alcohols, as a supercritical fluid for extracting components of natural products.

Conclusions

Experimental determinations of densities were carried out at the temperatures 313−363 K and at pressures up to 25 MPa for 1-propanol and 2-propanol, using a vibrating tube densimeter DTV. The reported data are consistent with those appearing in the literature, and the correlated models are reliable for extrapolating densities at lower temperatures.

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