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Article

Measurement of Liquid Density of Mixtures of 1-Propanol + 2-(2-Methoxyethoxy)ethanol at Temperatures from 298.15 to 393.15 K and Pressures up to 140 MPa and Modeling Using PC-SAFT and Peng−Robinson Equations of State

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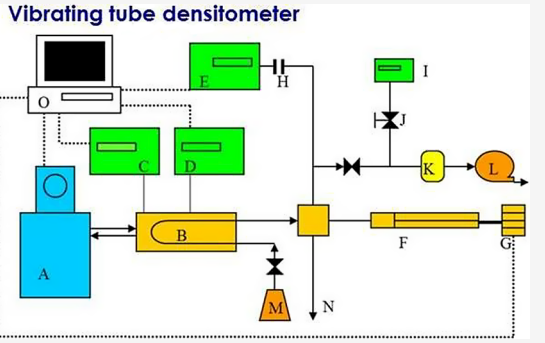
ABSTRACT: The environmental imperative driving the search for alternative fuels has fostered the rise of biofuels from biomass, offering renewable solutions that curtail petroleum dependence and greenhouse gas emissions. Propanol, as a primary biofuel, serves as an oxygenated additive, enhancing combustion efficiency and mitigating air pollutants. Propanol's oxygen-rich composition enhances engine performance and diminishes emissions. Studies on alkoxyethanols-gasoline blends showcase significant reductions in toxic pollutants, underscoring the need for thermodynamic understanding to foster cleaner energy. This study presents high-temperature and high-pressure density data for the binary mixture of 1-propanol, an alcohol, and 2-(2-methoxyethoxy)ethanol, an alkoxyethanol, covering temperatures ranging from 298.15 to 393.15 K and pressures from 0.1 to 140 MPa. The experimental density data were generated using a vibrating tube densitometer with an uncertainty of 0.7×10^{-3} g cm^{-3}. Experimental density data were fitted by using the Tait-like equation, with low standard deviations. Also, the experimental measurements were correlated using PC-SAFT and Peng−Robinson equations of state. The derived properties, such as excess volume, isobaric thermal expansivity, and isothermal compressibility, were also calculated.



1. INTRODUCTION

The necessity of finding alternative fuels has been driven by environmental concerns, leading to the emergence of biofuels as solutions to these challenges. Biomass, defined as the biodegradable fraction of products, waste, and residues from biological origins, serves as the primary source for biofuels originating from agriculture, forestry, and related industries. The use of biofuels as sources of renewable energy can decrease both the supply and consumption of petroleum, thereby reducing greenhouse gas emissions. Additionally, biofuels, such as ethanol, propanol, and methanol, serve as oxygenated fuel additives, enhancing combustion efficiency and reducing air pollutants like carbon monoxide and smog formation.[1,2]

Several studies[3,4] have been conducted to investigate mixtures of alkoxyethanols with gasoline, and the results have shown a significant reduction in the number of toxic pollutants such as CO emissions, hydrocarbons, and particulates. Furthermore, the findings of this research demonstrate that the addition of oxygen to alkoxyethanols is more convincing than the addition to alcohol. Indeed, incorporating alkoxyethanols into diesel fuel results in a decrease in viscosity properties while the oxidation stability of the fuel and Conradson carbon residues remains constant.[3] Alkoxyethanols are formed by combining the following three components: hydrocarbon, alcohol, and ether chains, with both nonpolar and polar properties, which provide versatile solvency characteristics. In fact, alkoxyethanols are used for various applications, primarily as industrial solvents. They are also used as additives in diesel fuel.[4]

2-(2-Methoxyethoxy)ethanol, also known by its trade name methyl carbitol,[5] belongs to the alkoxyethanols family and it can be used as a jet fuel anti-icing additive and as a solvent for the ink, dye, or painting industries. 2-(2-Methoxyethoxy)ethanol can also be used in coalescing blends with other solvents where high polymer solvency and tailing activities are needed.

This work is a continuation of our previously published research on the thermodynamic properties of mixtures composed of alkoxyethanols, hydrocarbons, and alcohols.[6−18]

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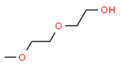
Table 1. Purity and Related Data of Chemicals

Compound	Chemical structure	Molar mass/g·mol^{-1}	Stated purity[a]/ mol %	CAS number
2-(2-Methoxyethoxy) ethanol		120.15	>99.0	111-77-3
1-propanol		60.10	>99.8[b]	71-23-8

[a]Determined by gas chromatography (GC) by the supplier Sigma-Aldrich. [b]The water content was checked to be less than 0.01% by the titration method.

In this work, we report new $p\rho T$ experimental data of the mixture 1-propanol + 2-(2-methoxyethoxy)ethanol at pressures up to 140 MPa and temperatures between 298.15 and 393.15 K. The isobaric thermal expansion and the isothermal compressibility for the same mixture are derived for six mole fractions. The experimental densities of the studied binary mixture of 1-propanol + 2-(2-methoxyethoxy)ethanol were correlated using the Tait-like equation and predicted using PC-SAFT and Peng−Robinson equations of state. One literature reference of Pal and Kumar[19] at 0.1 MPa and 308.15 and 318.15 K was found for the studied binary system.

2. EXPERIMENTAL SECTION

2.1. Materials. 1-Propanol and 2-(2-methoxyethoxy)-ethanol were supplied by Sigma-Aldrich. 1-Propanol presents a certified 0.998 mole fraction purity, while for 2-(2-methoxyethoxy)ethanol the certified mole fraction purity is greater than 0.990. Careful degassing before the use of both fluids was performed. The two fluids were used without any further purification. Data of chemicals are shown in Table 1.

2.2. Measurement Technique: Experimental Procedure. Density measurements were conducted using an Anton Paar DMA HPM vibrating tube densitometer. The density, ρ, was determined across a range of pressures (0.1−140 MPa) and temperatures (298.15−393.15 K). The operational and calibration methods for the device are documented in previous studies.[20] Calibration followed the procedures outlined by Comuñas et al.[21] and Lagourette et al.,[22] utilizing vacuum and water as reference fluids. The water density values were derived from the Wagner and Pruß[23] EoS. At p = 0.1 MPa and $T \geq$ 373.15 K, the use of decane as a calibrant was found convenient because its density at the atmospheric pressure over wide temperature intervals is reported by ref 24 with good accuracy. Temperature measurements were taken using a calibrated Pt 100 probe, with an estimated expanded uncertainty of 0.03 K. Pressure was measured with a WIKA CPH 6000 pressure transducer, with an estimated expanded uncertainty of 0.04 MPa. Both the temperature and pressure probes were calibrated prior to and following the measurements. The oscillation period of the vibrating cell was recorded by an Anton Paar mPDS 2000 V3 evaluation unit, which is connected to a DMA HPM densitometer. Considering the uncertainties in temperature, pressure, the oscillation period for water and vacuum, and the water density, the estimated expanded uncertainty (k = 2) for density is 0.7 × 10^{-3} g cm^{-3} (approximately 0.07% for densities near that of water), following the EA-4/02 document.[25] At a pressure of 0.1 MPa and a temperature of 373.15 K or higher, the uncertainty is estimated to be below 0.5%.

The pure fluids were degassed using a PSelecta Ultrason-H ultrasonic bath. Binary mixtures were prepared by weighing the components inside sealed glass vials to prevent evaporation using a Mettler Toledo MS2045 balance. This balance has a resolution of 10^{-4} g and an estimated expanded uncertainty of 0.0001 g. The estimated expanded uncertainty for the mole fraction is 5 × 10^{-4}. Consequently, the uncertainty in the excess molar volume is 0.004 cm^3 mol^{-1}.

3. MODELING

3.1. Tait-like Representation. To correlate density values across a wide range of temperatures and pressures, we utilized the Tait equation. This equation is commonly employed by experimental researchers for fitting high-pressure and high-temperature density data for pure compounds and mixtures. A key advantage of the Tait equation is its ability to provide excellent results not only for interpolating and fitting density data but also for derived properties such as isobaric expansion and isothermal compressibility. The authors have previously applied the Tait equation in their research,[20,26−30] and it is defined as

$$\rho(T, p) = \frac{\rho_0(T)}{1 - C\ln\left(\frac{B(T) + p}{B(T) + 0.1\ \text{MPa}}\right)} \quad (1)$$

where

$$\rho_0(T) = A_0 + A_1 T + A_2 T^2 + A_3 T^3 \quad (2)$$

$$B(T) = B_0 + B_1 T + B_2 T^2 \quad (3)$$

The parameters A_i, B_i, and C were determined by simultaneously correlating the experimental densities listed in Table 2 with both temperature and pressure. Consequently, Table 3 presents the results of the Tait equation correlation for the binary mixtures of x 1-propanol + (1 − x) 2-(2-methoxyethoxy)ethanol.

3.2. PC-SAFT EoS. The perturbed chain for statistical associating fluid theory (PC-SAFT) is an equation of state (EoS) that provides a thermodynamic model,[31,32] using hard chains formed by spherical particles as a reference fluid.

In PC-SAFT EoS the residual Helmholtz free energy $\breve{a}^{res}$ is fractionated into terms that account for various types of intermolecular interactions, namely, the hard chain reference $\breve{a}^{hc}$, the association interaction $\breve{a}^{assoc}$, and the dispersion interactions $\breve{a}^{disp}$.

$$\breve{a}^{res} = \breve{a}^{hc} + \breve{a}^{disp} + \breve{a}^{assoc} \quad (4)$$

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Table 2. Experimental Densities, ρ (g cm^{-3}), for the Binary Mixture of x 1-Propanol + $(1 - x)$ 2-(2-Methoxyethoxy)ethanol at Various Temperatures T and Pressures p[a]

x	p/MPa	T/K					
		298.15	313.15	333.15	353.15	373.15	393.15
ρ (g cm^{-3})							
0.0000	0.10	1.0153	1.0020	0.9841	0.9657	0.9468	0.9276
	1.00	1.0158	1.0026	0.9847	0.9664	0.9476	0.9284
	5.00	1.0182	1.0051	0.9875	0.9696	0.9511	0.9323
	10.00	1.0211	1.0082	0.9909	0.9733	0.9553	0.9370
	15.00	1.0240	1.0113	0.9943	0.9770	0.9593	0.9414
	20.00	1.0266	1.0142	0.9973	0.9805	0.9629	0.9457
	25.00	1.0293	1.0169	1.0005	0.9839	0.9667	0.9498
	30.00	1.0318	1.0198	1.0035	0.9872	0.9705	0.9537
	35.00	1.0345	1.0225	1.0064	0.9904	0.9740	0.9575
	40.00	1.0370	1.0250	1.0093	0.9932	0.9771	0.9611
	45.00	1.0394	1.0276	1.0121	0.9964	0.9804	0.9646
	50.00	1.0417	1.0301	1.0148	0.9993	0.9836	0.9680
	55.00	1.0441	1.0326	1.0174	1.0021	0.9867	0.9713
	60.00	1.0464	1.0350	1.0200	1.0048	0.9897	0.9746
	65.00	1.0486	1.0374	1.0226	1.0076	0.9926	0.9776
	70.00	1.0507	1.0398	1.0250	1.0103	0.9954	0.9807
	80.00	1.0551	1.0443	1.0298	1.0153	1.0009	0.9866
	90.00	1.0592	1.0486	1.0344	1.0203	1.0061	0.9922
	100.00	1.0633	1.0527	1.0389	1.0250	1.0112	0.9975
	110.00	1.0670	1.0568	1.0432	1.0296	1.0160	1.0026
	120.00	1.0711	1.0607	1.0473	1.0341	1.0207	1.0075
	130.00	1.0746	1.0646	1.0514	1.0383	1.0251	1.0122
	140.00	1.0783	1.0683	1.0553	1.0423	1.0295	1.0168
0.1511	0.10		0.9802	0.9623			
	1.00	0.9933	0.9809	0.9630	0.9446	0.9257	0.9064
	5.00	0.9957	0.9835	0.9659	0.9479	0.9295	0.9105
	10.00	0.9987	0.9866	0.9694	0.9518	0.9338	0.9154
	15.00	1.0016	0.9898	0.9728	0.9556	0.9379	0.9200
	20.00	1.0043	0.9927	0.9761	0.9592	0.9416	0.9244
	25.00	1.0071	0.9956	0.9792	0.9627	0.9456	0.9286
	30.00	1.0097	0.9985	0.9824	0.9661	0.9494	0.9326
	35.00	1.0124	1.0013	0.9852	0.9693	0.9530	0.9365
	40.00	1.0148	1.0039	0.9882	0.9723	0.9562	0.9403
	45.00	1.0174	1.0066	0.9911	0.9755	0.9597	0.9438
	50.00	1.0197	1.0091	0.9939	0.9784	0.9629	0.9473
	55.00	1.0222	1.0117	0.9965	0.9813	0.9660	0.9506
	60.00	1.0245	1.0140	0.9992	0.9841	0.9691	0.9540
	65.00	1.0268	1.0166	1.0018	0.9869	0.9721	0.9571
	70.00	1.0289	1.0189	1.0043	0.9897	0.9749	0.9603
	80.00	1.0333	1.0234	1.0092	0.9949	0.9805	0.9662
	90.00	1.0375	1.0279	1.0139	0.9999	0.9858	0.9719
	100.00	1.0417	1.0321	1.0183	1.0046	0.9909	0.9773
	110.00	1.0454	1.0362	1.0227	1.0093	0.9958	0.9825
	120.00	1.0495	1.0401	1.0269	1.0137	1.0005	0.9875
	130.00	1.0531	1.0440	1.0310	1.0180	1.0050	0.9922
	140.00	1.0567	1.0478	1.0350	1.0221	1.0094	0.9968
0.3260	0.10	0.9648	0.9517	0.9339			
	1.00	0.9654	0.9523	0.9345	0.9163	0.8972	0.8776
	5.00	0.9679	0.9550	0.9376	0.9197	0.9010	0.8820
	10.00	0.9710	0.9584	0.9413	0.9237	0.9056	0.8870
	15.00	0.9740	0.9616	0.9448	0.9277	0.9099	0.8919
	20.00	0.9768	0.9646	0.9481	0.9314	0.9138	0.8965
	25.00	0.9797	0.9676	0.9515	0.9350	0.9179	0.9008
	30.00	0.9824	0.9706	0.9546	0.9385	0.9219	0.9050
	35.00	0.9852	0.9735	0.9576	0.9418	0.9255	0.9091
	40.00	0.9877	0.9761	0.9607	0.9449	0.9289	0.9129
	45.00	0.9903	0.9788	0.9637	0.9481	0.9324	0.9165

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Table 2. continued

x	p/MPa	T/K					
		298.15	313.15	333.15	353.15	373.15	393.15
ρ (g cm^{-3})							
	50.00	0.9927	0.9815	0.9665	0.9512	0.9357	0.9201
	55.00	0.9952	0.9841	0.9692	0.9542	0.9389	0.9236
	60.00	0.9976	0.9865	0.9719	0.9571	0.9421	0.9271
	65.00	1.0000	0.9891	0.9746	0.9599	0.9451	0.9302
	70.00	1.0021	0.9915	0.9771	0.9627	0.9480	0.9335
	80.00	1.0066	0.9961	0.9821	0.9680	0.9537	0.9395
	90.00	1.0109	1.0006	0.9869	0.9731	0.9591	0.9453
	100.00	1.0152	1.0050	0.9914	0.9779	0.9643	0.9508
	110.00	1.0190	1.0091	0.9959	0.9827	0.9693	0.9561
	120.00	1.0231	1.0131	1.0001	0.9872	0.9741	0.9611
	130.00	1.0267	1.0171	1.0043	0.9914	0.9786	0.9659
	140.00	1.0304	1.0208	1.0083	0.9957	0.9831	0.9706
0.5018	0.10	0.9314	0.9184	0.9006			
	1.00	0.9320	0.9191	0.9014	0.8832	0.8640	0.8440
	5.00	0.9346	0.9220	0.9046	0.8867	0.8680	0.8487
	10.00	0.9379	0.9254	0.9084	0.8910	0.8728	0.8540
	15.00	0.9410	0.9288	0.9122	0.8951	0.8773	0.8592
	20.00	0.9440	0.9319	0.9156	0.8990	0.8815	0.8641
	25.00	0.9470	0.9350	0.9190	0.9027	0.8857	0.8686
	30.00	0.9497	0.9381	0.9223	0.9063	0.8898	0.8730
	35.00	0.9525	0.9411	0.9255	0.9098	0.8937	0.8771
	40.00	0.9552	0.9438	0.9286	0.9130	0.8971	0.8811
	45.00	0.9578	0.9466	0.9317	0.9163	0.9007	0.8849
	50.00	0.9603	0.9493	0.9346	0.9195	0.9041	0.8887
	55.00	0.9629	0.9520	0.9373	0.9225	0.9074	0.8921
	60.00	0.9654	0.9545	0.9401	0.9255	0.9107	0.8957
	65.00	0.9678	0.9571	0.9429	0.9284	0.9137	0.8990
	70.00	0.9700	0.9596	0.9455	0.9313	0.9168	0.9022
	80.00	0.9746	0.9643	0.9505	0.9366	0.9226	0.9085
	90.00	0.9789	0.9689	0.9554	0.9419	0.9281	0.9144
	100.00	0.9832	0.9733	0.9601	0.9468	0.9334	0.9200
	110.00	0.9871	0.9775	0.9645	0.9516	0.9384	0.9253
	120.00	0.9912	0.9816	0.9688	0.9562	0.9432	0.9305
	130.00	0.9950	0.9856	0.9731	0.9605	0.9478	0.9353
	140.00	0.9987	0.9894	0.9771	0.9647	0.9524	0.9400
0.6750	0.10	0.8929	0.8800	0.8625			
	1.00	0.8935	0.8808	0.8632	0.8450	0.8257	0.8053
	5.00	0.8963	0.8838	0.8666	0.8488	0.8301	0.8104
	10.00	0.8997	0.8874	0.8707	0.8533	0.8352	0.8161
	15.00	0.9030	0.8909	0.8746	0.8577	0.8400	0.8216
	20.00	0.9061	0.8942	0.8781	0.8617	0.8442	0.8267
	25.00	0.9091	0.8974	0.8818	0.8656	0.8487	0.8315
	30.00	0.9120	0.9007	0.8852	0.8694	0.8530	0.8361
	35.00	0.9150	0.9037	0.8884	0.8731	0.8570	0.8404
	40.00	0.9177	0.9066	0.8917	0.8763	0.8606	0.8446
	45.00	0.9204	0.9094	0.8949	0.8797	0.8643	0.8485
	50.00	0.9230	0.9122	0.8978	0.8829	0.8678	0.8524
	55.00	0.9256	0.9150	0.9007	0.8861	0.8712	0.8560
	60.00	0.9282	0.9176	0.9035	0.8891	0.8746	0.8596
	65.00	0.9306	0.9202	0.9063	0.8921	0.8777	0.8631
	70.00	0.9329	0.9227	0.9090	0.8951	0.8808	0.8664
	80.00	0.9375	0.9276	0.9142	0.9005	0.8868	0.8728
	90.00	0.9420	0.9322	0.9191	0.9059	0.8924	0.8788
	100.00	0.9464	0.9367	0.9238	0.9109	0.8977	0.8845
	110.00	0.9503	0.9410	0.9284	0.9157	0.9028	0.8899
	120.00	0.9545	0.9451	0.9327	0.9203	0.9077	0.8951
	130.00	0.9583	0.9492	0.9370	0.9248	0.9124	0.9001
	140.00	0.9621	0.9530	0.9411	0.9290	0.9170	0.9049

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Table 2. continued

x	p/MPa	T/K					
		298.15	313.15	333.15	353.15	373.15	393.15
ρ (g cm^{-3})							
1.0000[b]	80.00	0.8476	0.8383	0.8260	0.8133	0.8001	0.7862
	90.00	0.8523	0.8432	0.8312	0.8188	0.8059	0.7924
	100.00	0.8567	0.8477	0.8359	0.8238	0.8113	0.7983
	110.00	0.8608	0.8522	0.8405	0.8289	0.8166	0.8039
	120.00	0.8650	0.8564	0.8451	0.8336	0.8215	0.8091
	130.00	0.8689	0.8604	0.8493	0.8381	0.8264	0.8142
	140.00	0.8727	0.8645	0.8534	0.8424	0.8309	0.8190

[a]Estimated expanded uncertainties (k = 2): temperature, $U(T)$ = 0.03 K; pressure, $U(P)$ = 0.04 MPa; density, $U(\rho) = 0.7 \times 10^{-3}$ g cm^{-3}; mole fraction, $U(x) = 5 \times 10^{-4}$. [b]Experimental high-pressure density data for 1-propanol along the six temperatures (interval 298.15−393.15 K) and 16 pressures (interval 0.1−70 MPa) have already been published by Muñoz-Rujas et al.[73]

Table 3. Obtained Parameters and Deviations for Density Correlation by Using Eqs 1−3 for x 1-Propanol + $(1 - x)$ 2-(2-Methoxyethoxy)ethanol

parameters	x					
	0.0000	0.1511	0.1511	0.1511	0.1511	1.0000
A_0/g cm^{-3}	1.2679	0.96890	1.2223	1.2012	1.1986	1.3311
A_1/g cm^{-3} K^{-1}	-9.0995×10^{-4}	1.4289×10^{-3}	-1.0224×10^{-3}	-1.1779×10^{-3}	-1.5629×10^{-3}	-3.7889×10^{-3}
A_2/g cm^{-3} K^{-2}	5.1629×10^{-7}	-6.0306×10^{-6}	1.0592×10^{-6}	1.6577×10^{-6}	2.9920×10^{-6}	1.0206×10^{-5}
A_3/g cm^{-3} K^{-3}	-1.0263×10^{-9}	5.0538×10^{-9}	-1.7652×10^{-9}	-2.4885×10^{-9}	-3.9860×10^{-9}	-1.1659×10^{-8}
B_0/MPa	515.09	504.74	462.61	430.26	389.51	300.66
B_1/MPa K^{-1}	−1.6055	−1.6071	−1.4349	−1.3326	−1.1836	−0.85493
B_2/MPa K^{-2}	1.2895×10^{-3}	1.3249×10^{-3}	1.1188×10^{-3}	1.0200×10^{-3}	8.5504×10^{-4}	4.9307×10^{-4}
C	0.08894	0.088826	0.089132	0.088966	0.088989	0.088972
AAD[a]/%	0.006	0.009	0.006	0.006	0.007	0.010
MD[b]/%	0.022	0.022	0.023	0.023	0.027	0.030
σ[c]/g cm^{-3}	7.76×10^{-5}	1.05×10^{-4}	7.62×10^{-5}	7.46×10^{-5}	8.30×10^{-5}	9.61×10^{-5}
RMSD[d]/g cm^{-3}	7.54×10^{-5}	1.02×10^{-4}	7.39×10^{-5}	7.42×10^{-5}	8.05×10^{-5}	9.32×10^{-5}

[a]Absolute average deviation, AAD = $\frac{100}{N}\sum_{i=1}^{N}\left|\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}}\right|$. [b]Maximum deviation, MD = Max$\left(100\left|\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}}\right|\right)$. [c]Root-mean-square deviation, RMSD = $\sqrt{\frac{\sum_{i=1}^{N}(\rho_i^{exp} - \rho_i^{calc})^2}{N}}$. [d]Standard seviation, $\sigma = \sqrt{\frac{\sum_{i=1}^{N}(\rho_i^{exp} - \rho_i^{calc})^2}{N - m}}$; N is the number of experimental data; m is the number of parameters (8 parameters).

Initially, Wertheim and Chapman[33−36] defined hard chains reference term, noted as $\breve{a}^{hc}$, as constituted by $\bar{m}$ segments, and analytically defined as

$$\breve{a}^{hc} = \bar{m}\breve{a}^{hc} - \sum_{i=1}^{n_c} x_i(m_i - 1)\ln g_{ij}^{hs} \quad (5)$$

where x_i is the molar fraction of the chain of compound i, m_i is the number of segments in the chain, and g_{ij}^{hs} is the radial distribution function for the segments of compound i in a system of hard spheres.

Second, the association interaction expression was defined by Chapman and Huang.[36,37] In fact, this term is mostly expressed as follows:

$$\breve{a}^{assoc} = \sum_{i=1}^{n_c} x_i\left[\sum_{A_i}\left(\ln X^{A_i} - \frac{X^{A_i}}{2}\right) + \frac{1}{2}M_i\right] \quad (6)$$

where M_i is the association sites number on each molecule, X^{A_i} is the composition of molecules I not linked at site A, and $\sum_{Ai}$ is a sum of all associating sites on each molecule.

Third, the dispersion interaction term, $\breve{a}^{disp}$, of the PC-SAFT equation has been defined by Barker and Henderson's perturbation theory.[38,39] For this part, the Helmholtz energy for dispersion is indicated as follows:

$$\breve{a}^{disp} = -2\pi\breve{\rho}I_1\overline{m^2\varepsilon\sigma^3} - \pi\breve{\rho}C_1I_2\overline{m^2\varepsilon^2\sigma^3} \quad (7)$$

where C_1 is the coefficient that depends on the mean segment number $\bar{m}$ and on the density number of fluid ρ and the perturbation integrals I_1 and I_2.

The equation of state (PC-SAFT) is described by non-associative parameters defining the segment number (m), the segment energy parameter (ε/k), and the segment diameter (σ). However, if the solution is nonideal, the association interaction term has to be split in eq 4 with two other parameters, the association volume (k^{AiBi}) and the association energy (ε^{AiBi}).

The PC-SAFT parameters of the studied binary system were found by utilizing the objective function, noted as Obj. F:

$$\text{Obj. F} = \sum_{i=1}^{N}\left(\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}}\right) \quad (8)$$

with N denoting the number of experimental data which was used in the fitting.

3.3. Peng−Robinson EoS. Based on Peng−Robinson[40] EoS for a pure fluid, the pressure p is expressed as a function of the temperature T and molar volume v:

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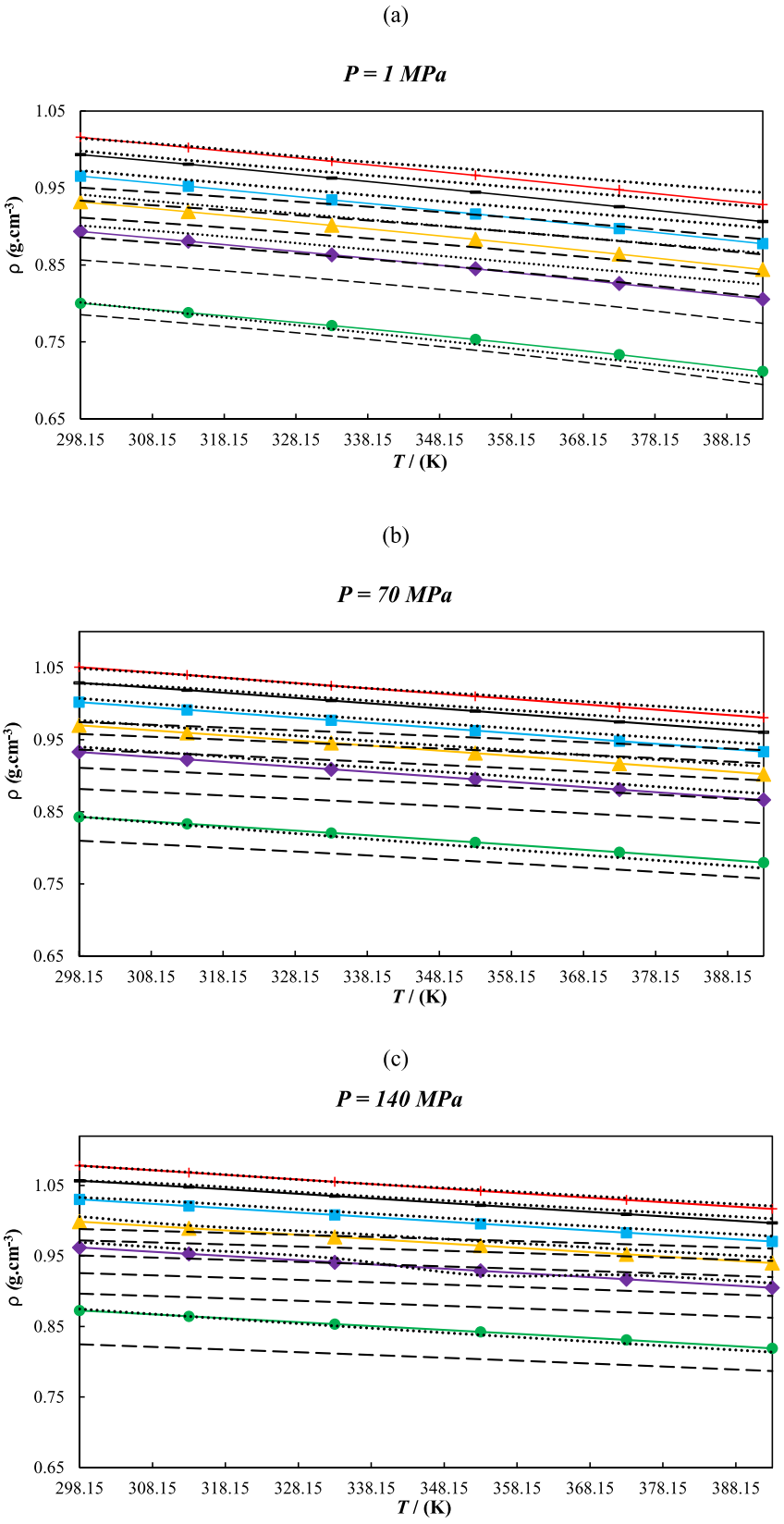

Figure 1. Experimental values of densities, ρ, for the binary mixture [1-propanol (1) + 2-(2-methoxyethoxy)ethanol (2)]: (a) at 1 MPa, (b) at 70 MPa, and (c) at 140 MPa: (red plus symbol), pure compound 2-(2-methoxyethoxy)ethanol, (green circle), pure compound 1-propanol, (purple diamond), $x_1 = 0.1511$, (yellow triangle), $x_2 = 0.3260$, (blue square), $x_3 = 0.5018$, (black dash), $x_4 = 0.6750$; (black line) Tait-like equation, (dotted line) PC-SAFT equation, and (dashed line) Peng–Robinson equation.

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Table 4. Characteristic Parameters of the PC-SAFT Model for 2-(2-Methoxyethoxy)ethanol and 1-Propanol

compound	m (−)	σ (A)	ε/k (K)	ε^{HB}/k (K)	K^{HB} (K)	AAD % (ρ^{Liq})
2-(2-methoxyethoxy)ethanol	5.82427	3.05987	245.707	0.105827	3767.82	0.04
1-propanol	2.6002	3.37781	275.455	0.01001	1040.45	0.05

$$p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2vb - b^2} \tag{9}$$

where R is the gas constant, and a and b are component-dependent parameters related to attractive and repulsive interactions, respectively, defined as

$$b = \frac{0.007780RT_c}{p_c} \tag{10}$$

$$a = a(T_c)[1 + k(1 - T_r^{0.5})]^2 \tag{11}$$

$$a(T_c) = \frac{0.45724R^2T_c^2}{p_c} \tag{12}$$

$$k = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{13}$$

where P_c is the critical pressure, T_c is the critical temperature, and k is dependent on the acentric factor ω:

$$\omega = -\log\left(\frac{p}{p_c}\right)_{T/T_c=0.7} - 1 \tag{14}$$

Note that P_c, T_c, and ω data for the pure components studied, 1-propanol and 2-(2-methoxyethoxy)ethanol, are sourced from the work reported by Yaws.[41]

For the application of Peng−Robinson EoS, the coefficients a_{mix} and b_{mix}, are determined using van der Waals law mixing rules:

$$a_{mix} = \sum_i \sum_j x_i x_j a_{ij} \tag{15}$$

$$b_{mix} = \sum_i x_i b_i \tag{16}$$

$$a_{ij} = (a_{ii}a_{jj})^2(1 - K_{ij}) \tag{17}$$

where K_{ij} is the binary interaction parameter between components i and j, generally supposed to be equal to zero and x_i is the mole fraction of component i.

4. RESULTS AND DISCUSSION

4.1. Density. The measured densities of the binary mixtures of x 1-propanol + $(1 - x)$ 2-(2-methoxyethoxy)ethanol (molar compositions, x = 0.0000, 0.1511, 0.3260, 0.5018, 0.6750, and 1.0000) along the 6 temperatures (interval 298.15−393.15 K) and 23 pressures (interval 0.1−140 MPa) are reported in Table 2. Because of the 1-propanol boiling point (T = 370.03 K), density measurements at p = 0.1 MPa were limited to T = 333.15 K for the binary systems. It is important to note that the experimental high-pressure density data for the pure component 1-propanol at temperatures ranging from 298.15 to 393.15 K and pressures ranging from 0.1 to 70 MPa have already been published by Muñoz-Rujas et al.[73]

Figure 1a−c describes the evolution of both the measured and the calculated densities using the three equations, Tait-like, PC-SAFT, and Peng−Robinson as a function of temperature at (a) p = 1 MPa, (b) at p = 70 MP and p = 140 MPa, at each composition. These figures reveal that the density of x 1-propanol + $(1 - x)$ 2-(2-methoxyethoxy)ethanol decreases when the temperature increases and increases when the pressure increases. This nonlinear behavior of density with temperature (particularly at low pressure) justifies the use of eq 2, as shown by Figure 1a. Overall, it is evident that the logarithmic Tait-type equation is very much adequate to represent the dependence of density with respect to pressure, as shown by the shape of the isothermal curves. Regarding the influence of mole fraction, Figure 1 demonstrates that the density of the binary mixture decreases as the mole fraction of 1-propanol increases.

Table 3 reports the Tait-like equation parameters along with the absolute average deviation (AAD), maximum deviation (MD), root-mean-square deviation (RMSD), and the standard deviation (σ) between ρ_{exp} and ρ_{calc} for our binary mixture. Note that all of the deviation parameters listed in Table 3 are lower than the experimental uncertainty, indicating a good correlation of the data.

Table 4 presents the PC-SAFT parameters for the pure components 1-propanol and 2-(2-methoxyethoxy)ethanol. The AADs of 1-propanol and 2-(2-methoxyethoxy)ethanol were 0.05% and 0.04%, respectively. Table 5 lists the critical parameters (critical temperature T_c, critical pressure P_c, acentric factor ω) required for the Peng−Robinson EoS.

Table 5. Critical Temperature T_c, Critical Pressure P_c, and Acentric Factor ω of Pure Components 2-(2-Methoxyethoxy)ethanol and 1-Propanol

compound	T_c	P_c	ω	refs
2-(2-methoxyethoxy)ethanol	630.00	35.45	0.635	41
1-propanol	536.78	51.75	0.622	41

Figure 2 presents the percentage deviations between the predicted density data of 1-propanol using PC-SAFT parameters reported in this work and those reported previously in the literature.[42−45] The maximum deviation is obtained by Paduszynski et al.[43] (AAD = 2.37%), followed by Grenner et al.[44] and Waston et al.[45] with an AAD equal to 1.61 and 0.94%, respectively, and finally the lower deviation is acquired by Liang et al.[42] (AAD = 0.82%). The maximum deviation obtained by our PC-SAFT parameters is 1.18%.

The absolute average deviation (AAD) is computed to compare the experimental with the predicted data that are provided by the Tait-like equation, PC-SAFT, and Peng−Robinson equations of state. The Tait-like equation is a mathematical equation widely employed to fit liquid density data over large pressure and temperature ranges. In fact, the highest AAD found for the pure component 2-(2-methoxyethoxy)ethanol, where x = 0, is 0.006%. As well as for 1-propanol, where x = 1, the maximum AAD determined is 0.01%. The experiment was performed with four various fractions of the mixture. For x_1 = 0.1511, x_2 = 0.3260, x_3 = 0.5018, x_4 = 0.6750, the maximum AAD found by calculation is respectively 0.009, 0.006, 0.006, and 0.007% all over the studied temperature range. The same analysis was accomplished using

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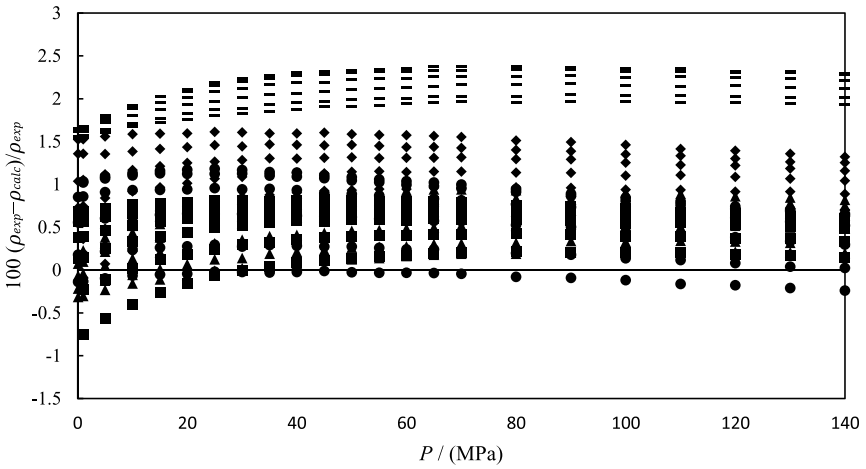

Figure 2. Percentage deviations versus pressure of densities for 1-propanol: (circle) using our estimated PC-SAFT parameters, (square) Liang et al.;[42] (dashed line) Paduszynski et al.;[43] (diamond) Grenner et al.;[44] (triangle) Waston et al.[45]

Table 6. Literature Comparison between the Values Generated Using the Tait-like Equation at Exactly the Same Experimental *p*, *T* Sets Given for 1-Propanol and 2-(2-Methoxyethoxy)ethanol at High Pressure for Several Literature References[a]

reference	year	N_p	T_{min}/K	T_{max}/K	P_{min}/MPa	P_{max}/MPa	AAD/%	MD/%	Bias/%
1-propanol									
Kubota et al.[48]	1987	27	283.15	348.15	0.10	207.60	0.06	0.13	−0.05
Ormanoudis et al.[49]	1991	11	288.15	308.15	0.10	33.81	0.04	0.05	−0.05
Papaioannou et al.[50]	1993	10	298.15	298.15	0.10	33.90	0.05	0.07	−0.05
Papaioannou and Panayiotou[51]	1995	10	298.15	298.15	0.10	33.90	0.06	0.09	−0.06
Yaginuma et al.[52]	1998	12	313.15	313.15	0.10	9.80	0.07	0.10	0.04
Zúñiga-Moreno and Galicia-Luna[53]	2002	164	313.15	362.77	0.50	25.09	0.08	0.12	0.08
Kitajima et al.[54]	2003	16	315.15	430.15	5.118	26.008	0.03	0.04	−0.03
Gil-Hernández et al.[55]	2005	20	288.15	308.15	0.10	19.70	0.05	0.14	−0.04
Zéberg-Mikkelsen and Andersen[56]	2005	28	303.15	333.15	0.10	30.00	0.04	0.11	0.04
Watson et al.[45,57]	2006	84	293.15	353.15	0.10	65.00	0.04	0.09	0.001
Abdulagatov et al.[58]	2008	36	298.15	423.15	0.11	39.95	0.04	0.11	0.04
Torcal et al.[59]	2010	15	283.15	328.15	0.10	20.00	0.03	0.09	−0.02
Torcal et al.[60]	2010	15	283.15	328.15	20.00	40.00	0.04	0.09	0.04
Dávila et al.[61]	2012	98	278.15	358.15	0.10	60.00	0.12	0.21	0.12
Kariznovi et al.[62]	2013	22	302.20	323.20	0.10	10.00	0.07	0.12	−0.02
Alaoui et al.[63]	2014	60	293.15	353.15	0.10	140.00	0.02	0.08	0.001
2-(2-methoxyethoxy)ethanol									
López et al.[64]	2004	54	283.15	353.15	0.10	25.00	0.02	0.05	0.001

[a] N_p represents the number of data points which are in our *p*, *T* ranges.

the equation of state PC-SAFT. For 2-(2-methoxyethoxy)-ethanol as a pure constituent, the AAD calculated varies from the lowest value of 0.04% at 313.15 K and the highest value of 0.92% at 393.15 K. In addition, for 1-propanol, the minimum AAD value is 0.08% found at 298.15 K and the maximum AAD is 0.96% at 393.15 K. Regarding the experiment with different fractions. For x_1 = 0.1511, x_2 = 0.3260, x_3 = 0.5018, and x_4 = 0.6750, the AAD values determined by calculation are respectively varying over the following ranges [0.34%; 1.10%], [0.55%; 1.30%], [0.72%; 1.40%] and [0.69%; 1.25%] all over the studied temperature range. Besides, the same calculation was done by the Peng−Robinson equation of state. For 2-(2-methoxyethoxy)ethanol, the AAD extends from 4.71% at 393.15 K to 7.11% at 298.15 K. For 1-propanol as a pure component, the AAD goes from 2.68% at 393.15 K to 3.46% at 298.15 K. The AAD values were also calculated with the Peng−Robinson equation for various fractions of the studied binary mixture. For x_1 = 0.1511, x_2 = 0.3260, x_3 = 0.5018, and x_4 = 0.6750, the AAD values determined are respectively varying over the following ranges [4.37%; 6.47%], [4.19%; 6.38%], [3.95%; 5.86%] and [3.65%; 5.21%] all over the studied temperature range. In fact, the Tait-like equation gives interesting results, because it is a mathematical equation that uses various parameters to fit the experimental data. Also, the PC-SAFT equation shows advantageous results compared to the Tait equation and Peng−Robinson equation. Considering that the PC-SAFT equation accounts for both inter- and intramolecular interactions in the studied mixture and is based on statistical mechanics, which takes into consideration the size and shape of the molecules, it provides a robust framework for predicting the behavior of complex mixtures. Additionally, the explicit consideration of molecular association in PC-SAFT[46,47] further enhances its accuracy in modeling such systems. However, the Peng−Robinson as Cubic state equation gives the worst fit to the experimental data with higher AAD values, compared to the other models.

4.2. Comparison with Literature Data. Several available density data sets for 1-propanol and 2-(2-methoxyethoxy)-

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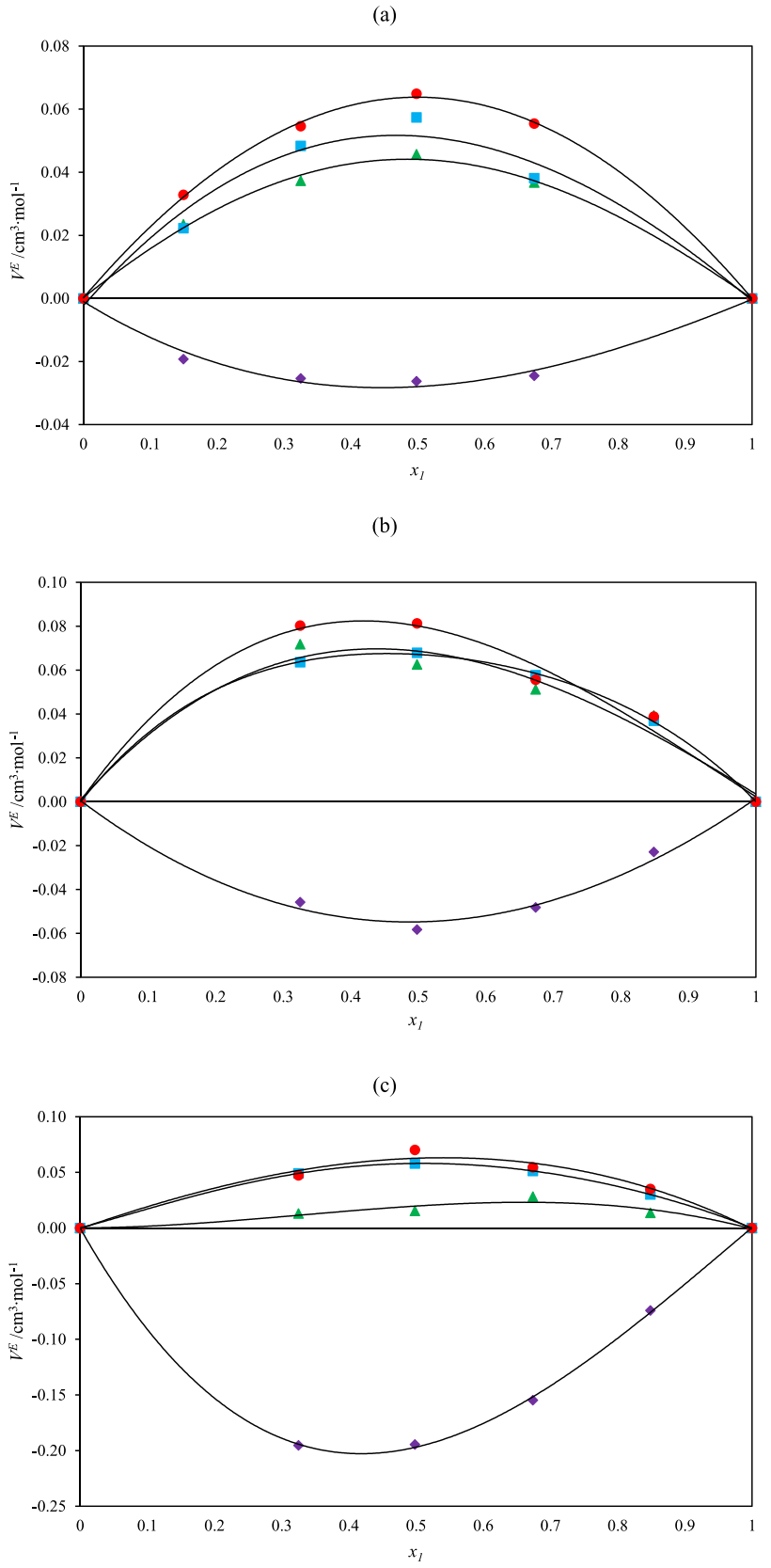

Figure 3. Experimental values of excess molar volumes for the mixtures of x 1-propanol + (1-x) 2-(2- methoxyethoxy) ethanol as a function of the mole fraction at different temperatures: (a) at T = 298.15 K, (b) at T = 353.15 K, and (c) at T = 393.15 K, where purple diamond, 1 MPa; green triangle, 50 MPa; blue square, 100 MPa; red circle, 140 MPa; (black line), Redlich−Kister's eq 19.

ethanol at high pressure have been previously published in the literature, and these are presented in Table 6. Note that this list is not exhaustive. In Table 6, N_P represents the number of data points that fall within our pressure and temperature intervals.

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We have compared the experimental density data reported in the literature with the values predicted by our correlation (eqs 1−3 and Table 3), ensuring that the pressure and temperature sets are within our experimental intervals to avoid any extrapolation.

The density of 1-propanol at high pressure has been measured by several authors.[45,48−64] Agreement with most sets of reference data[48,51,52,62] is quite good as the AAD is similar to our experimental uncertainty and is excellent for the most part of references[45,49,50,54−60,63] as the AAD is well under our experimental uncertainty. The comparison with reference[53] (claimed uncertainty 0.05%) shows an AAD of 0.08%, only slightly higher than our experimental uncertainty. Finally, the comparison with data of reference[61] (claimed uncertainty 1.2 kg m^{-3}) shows a quite significant deviation, with bias = 0.12%. Notice that these authors used for their calibration procedure both water (whose density is very well-known) and hexane (whose density accuracy is only 0.2%, quite poor for reference compounds).

Concerning the density of pure 2-(2-methoxyethoxy)ethanol at high pressure, only one reference was found,[64] reporting data up to 25 MPa in the interval (283.15 to 353.15) K. The agreement between this set of data and our correlation is excellent, showing an AAD of 0.02% and an MD of 0.05, well below our estimated uncertainty.

Only one set of density data for the binary system of 1-propanol + 2-(2-methoxyethoxy)ethanol within our pressure and temperature intervals has been found, specifically at 0.1 MPa and at temperatures of 308.15 and 318.15 K.[19]

4.3. Excess Volumes. The excess volume, V^E, was calculated using the following equation:

$$V^{\mathrm{E}} = \sum_{i=1}^{n} x_i M_i [(1/\rho) - (1/\rho_i)] \tag{18}$$

with n: the number of components; x_i: the composition of component i in the mixture; M_i: the molar mass; while ρ and ρ_i are the experimental densities of the studied binary mixture and pure component i, respectively. The density of pure 1-propanol and pure 2-(2-methoxyethoxy)ethanol is reported in Table 2, and they are used for the calculation of V^{E}.

Using eq 18, the V^{E} values of the studied binary mixture 1-propanol +2-(2-methoxyethoxy)ethanol were calculated. The V^{E} of studied binary mixtures as a function of pressure are illustrated in Figure 3a,b. It is clearly observed that the V^{E} values are negative at initial pressures, but from 50 MPa, it can be noticed that the trend in the V^{E} values is positive and becomes more positive with increasing pressure. The interactions between polar components 1-propanol (alcohol) and 2-(2-methoxyethoxy)ethanol (alkoxyethanol) are suggested by the formation of hydrogen bonds between the two molecules. The strength of interactions between 1-propanol and 2-(2-methoxyethoxy)ethanol can differ from those in the pure solvents (i.e., alcohol−alcohol), influenced by their functional groups' hydrogen-bonding capabilities. If the hydrogen bonds in the mixture are stronger than in the pure solvents, negative deviations from ideal behavior occur, indicating stronger attractions. Weaker hydrogen bonds lead to positive deviations, reflecting weaker interactions. These deviations underscore the complexity of the molecular interactions in the mixture. In addition, Figure 3 shows that the V^{E} decreases with increasing temperature, which means that there is a strong interaction between different molecules than molecules of the same nature and therefore a strong packing effect.[65−69] The increase in pressure increases proportionally the V^{E}, which is translated by the weakening of the packing effect due to the disorder in the orientation order or breaking of cohesion forces between the straight chain of two molecules.

The V^{E} of the binary mixture 1-propanol + 2-(2-methoxyethoxy)ethanol, was fitted by the Redlich−Kister equation (Figure 3 and Table 7):

$$V^{\mathrm{E}} = x(1-x)\sum_i z_i(2x-1)^{i-1} \tag{19}$$

Table 7. Values of Parameters z_i of Eq 19 and the Corresponding Standard Deviation, σ, for Binary Mixtures of x 1-Propanol + $(1-x)$ 2-(2-Methoxyethoxy)ethanol at 298.15 and 393.15 K for Different Pressures and at 1.00 and 140.00 MPa for All the Temperatures Measured

	z_1	z_2	z_3	$\sigma\,(V^{\mathrm{E}})$/cm^3 mol^{-1}
p/MPa	(T = 298.15 K)			
0.10	−0.1193	0.0134	0.0086	0.001
1.00	−0.1327	−0.0897	−0.0909	0.001
10.00	−0.0511	0.0061	0.1370	0.003
25.00	0.1065	0.0794	0.0587	0.001
50.00	0.1719	0.0764	0.0268	0.001
100.00	0.2329	0.0583	0.0104	0.002
p/MPa	(T = 393.15 K)			
1.00	−0.7877	−0.2804	0.0018	0.002
10.00	−0.4156	−0.1917	−0.1586	0.001
25.00	−0.0991	−0.0887	0.0006	0.001
50.00	0.0801	−0.0773	−0.0129	0.004
100.00	0.2206	−0.0329	−0.0131	0.000
T/K	(p = 1.00 MPa)			
298.15	−0.1862	−0.1578	1.1933	0.017
313.15	−0.1284	0.0020	0.1483	0.002
333.15	−0.1298	−0.0592	0.0358	0.007
T/K	(p = 140.00 MPa)			
298.15	0.1757	−0.1097	1.2120	0.018
313.15	0.2663	0.0582	0.0433	0.002
333.15	0.2577	0.0605	0.0018	0.001
353.15	0.3070	0.1394	0.1430	0.004
373.15	0.2994	0.0377	0.0635	0.002
393.15	0.2629	−0.0692	−0.1247	0.004

where x is the mole fraction of 1-propanol and z_i are the parameters of the Redlich−Kister equation. The parameters z_i of the Redlich−Kister equation and the deviations were obtained at several pressures for temperatures T = (298.15 and 393.15) K and at several temperatures for pressures at p = (1 and 140) MPa.

4.4. Derived Thermodynamic Properties. Among the derived thermodynamic properties that can be derived from the densities, we find the thermal compressibility and the isobaric thermal expansivity, they can give a valuable information than the density itself on the volumetric properties' dependence with respect to temperature T and pressure p.

The isothermal compressibility, κ_T, which reflects the effect of pressure on density and is calculated using the Tait equation, as given by the following equation:

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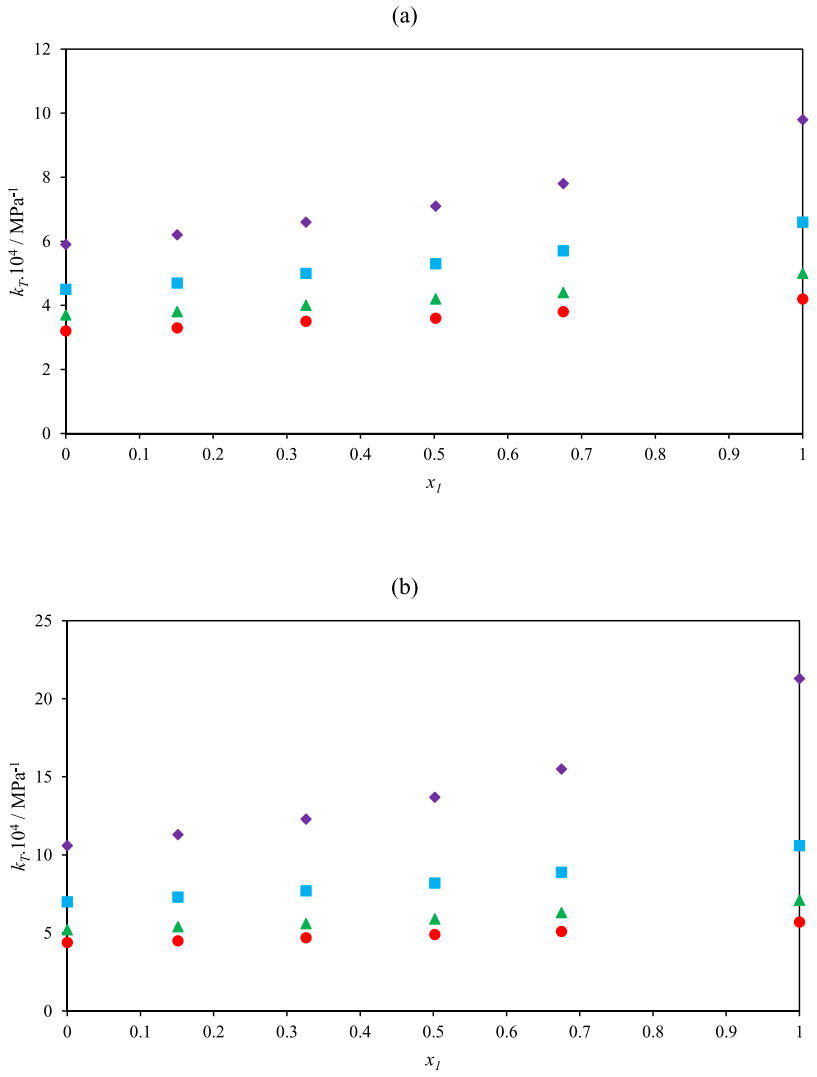

Figure 4. Isothermal compressibility, 104 κ_T, for x 1-propanol + $(1 - x)$ 2-(2-methoxyethoxy)ethanol as a function of the mole fraction at different temperatures: (a) at T = 298.15 K and (b) at T = 393.15 K, where purple diamond, 1 MPa; blue square, 50 MPa; green triangle, 100 MPa; red circle, 140 MPa.

$$\kappa_T = \left(\frac{1}{\rho}\right)\left(\frac{\partial \rho}{\partial p}\right)_T = \frac{C}{\left(1 - C\ln\left(\frac{B(T)+p}{B(T)+0.1\ \text{MPa}}\right)\right)\left(B\left(T\right)+p\right)} \quad (20)$$

Additionally, the isobaric thermal expansivity, α_p, can be obtained by deriving the density with respect to the temperature at constant pressure:

$$\alpha_p = -\left(\frac{1}{\rho}\right)\left(\frac{\partial \rho}{\partial T}\right)_p \quad (21)$$

However, the estimated isobaric thermal expansivity could be influenced by the form of functions $B(T)$ and $\rho_0(T)$, as cited by refs 70 and 71. Additionally, ref 72 points out that the values reported for the isobaric thermal expansivity could vary not only due to differences in density values but also to the fitting equation used. This temperature influence can be considered to more properly derive the isobaric densities. Therefore, at each pressure p, we suppose that $\rho_p(T) = a_0 + a_1T + a_2T^2$ and then $(\partial\rho/\partial T)_p = a_1 + 2a_2T$, and we get a set (a_0, a_1, a_2) for each pressure p.

As a result, by integrating the differentiated density data and incorporating the estimated densities $\rho_p(T)$ into the equation $\alpha_p = -(1/\rho(\partial\rho/\partial T)_p$, under different T, p conditions, the isobaric thermal expansivity is obtained:

$$\alpha_p = -\frac{a_1 + 2a_2T}{a_0 + a_1T + a_2T^2} \quad (22)$$

The calculated values of isothermal compressibility, κ_T, are presented in Figure 4 and listed in Table S1. Similarly, the calculated values of isobaric thermal expansivity, α_p, are shown in Figure 5 and detailed in Table S2. As shown in Figures 4 and 5, the increase in pressure leads to a decrease of κ_T and α_p. In the reverse, the increase in temperature leads to an increase of κ_T and α_p. These trends are the expected ones compared with the behavior of a large number of substances. For the isothermal compressibility, the estimated uncertainty is 0.001, while or the isobaric thermal expansivity reaches 0.003.

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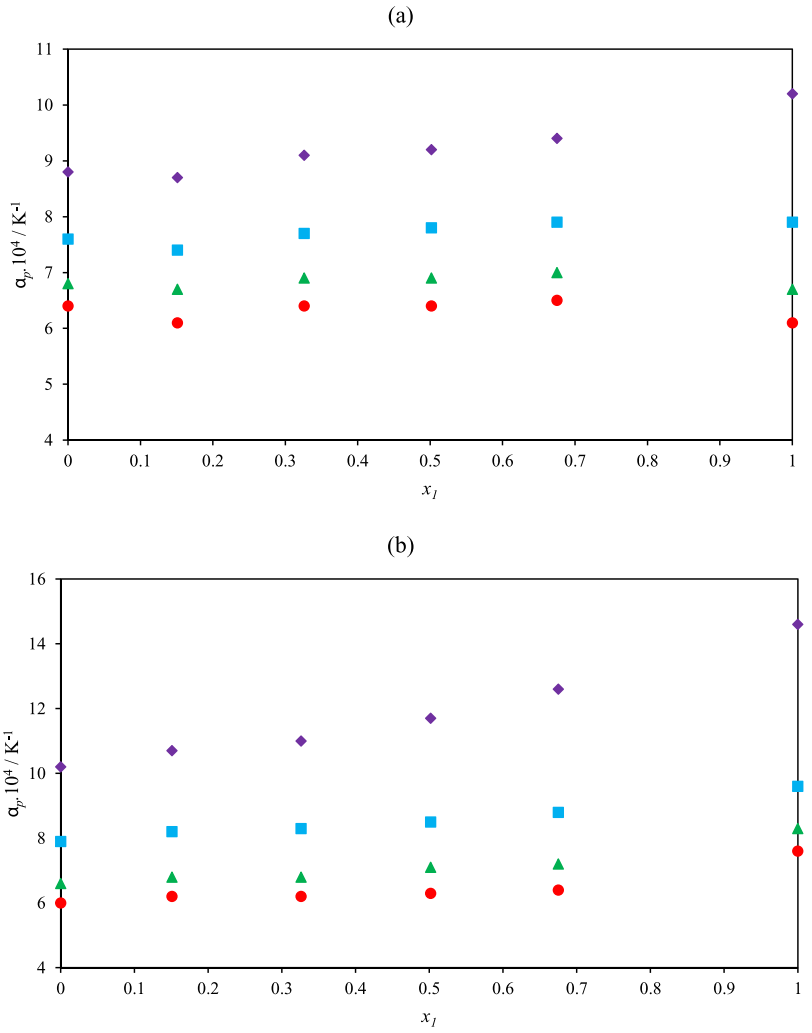

Figure 5. Isobaric thermal expansion coefficient 104 α_p, for x 1-propanol + $(1 - x)$ 2-(2-methoxyethoxy)ethanol as a function of the mole fraction at different temperatures: (a) at T = 298.15 K and (b) at T = 393.15 K, where purple diamond, 1 MPa; blue square, 50 MPa; green triangle, 100 MPa; red circle, 140 MPa.

5. CONCLUSIONS

New experimental densities for the binary mixture of 1-propanol +2-(2-methoxyethoxy)ethanol in the compressed liquid state were reported in this work. Measurements were performed over a temperature range of 298.15−393.15 K and a pressure range of 0.1−140 MPa. No literature references were found for the same temperature and pressure ranges for the studied binary mixture. The experimental density data were fitted and correlated using three equations: the Tait-like equation, PC-SAFT, and Peng−Robinson EoS. The Tait-like equation demonstrated the best fit with a maximum average absolute deviation (AAD) of 0.01. Derived thermodynamic properties, such as excess volume, isothermal compressibility, and isobaric thermal expansivity, were also calculated and are presented in this work.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jced.4c00232.

Isothermal compressibility and isobaric thermal expansion coefficient (PDF)

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Notes

The authors declare no competing financial interest.

LIST OF SYMBOLS

AAD	absolute average deviation
a_i	coefficients of isobaric thermal expansivity correlation
A_i, B_i, C	coefficients of density correlation
Bias	average deviation
calc	calculated
exp	experimental
i	constituent identification
lit	literature
MD	maximum deviation
N_P	number of experimental data points which are in our p, T ranges
p	pressure
p_0	reference pressure
RMSD	root-mean-square deviation
T	temperature
V^E	excess molar volume
EoS	equation of state

Greek Letters

σ	standard deviation
α_p	isobaric thermal expansivity
ρ	density
ρ_0	density at a reference pressure p_0
κ_T	isothermal compressibility

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