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Article

Thermophysical Study on the Mixing Properties of Mixtures Comprising 2-(2-Methoxyethoxy)ethanol, Butan-1-ol, Butan-2-ol, and Propan-1-ol

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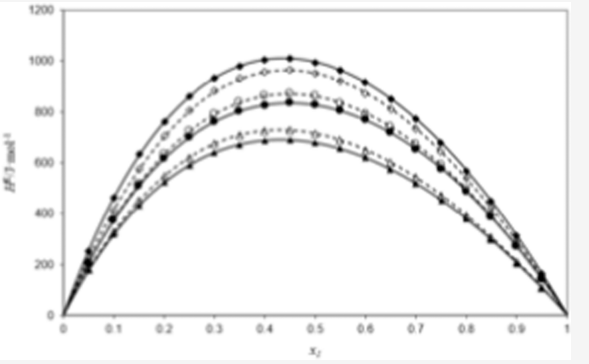
ABSTRACT: Excess enthalpy (H^E), dynamic and kinematic viscosities (η, υ), density (ρ), and refractive index (n_D) of mixtures comprising 2-(2-methoxyethoxy)ethanol, butan-1-ol, butan-2-ol, and propan-1-ol are presented at p = 0.1 MPa and at T = 298.15 and 313.15 K. Deviations in refractive index (Δn_D) is generated from experimental data of refractive index. Experimental data of ρ for all binary mixtures are predicted using the PC-SAFT (Perturbed Chain-Statistical Associating Fluid) EoS. Furthermore, H^E and Δn_D are adjusted using the Redlich−Kister equation. However, the correlation of measured data of H^E is performed by using the UNIQUAC and NRTL models.



1. INTRODUCTION

Conventional oil-based motor fuels currently provide many energy needs for the mobility of people and goods. Gasoline and diesel cover 98% of the energy used in the transport sector on a global scale, and 96% in Europe where biofuels represent only 1.5% and natural gas just over 1%.[1] Energy consumption in the transport sector is increasing at an annual rate of around 2%. Many improvements have been applied on the traditional fuels (cetane and octane numbers, sulfur, lead content, etc.) to reach higher specifications and still need to be improved to realize the future specifications already programmed. While the transport sector is more than 98% dependent on oil products, in the context of high fuel costs and combating GHG emissions, alternative energies are multiplying, and many sectors follow one another to replace petroleum fuels. In the same context, several studies have shown that biofuels are the best renewable alternative to fossil fuels, which are generated directly from the plants. The majority of gasoline is mixed with biofuels such as bioethers and ethanol. Oxygenated gasoline additives like alcohols, ethers, and glycol ethers are used to yield positive results through their ability to increase the octane rating and to reduce the pollutants and the contaminant toxicity.[2,3] Our investigation of the thermophysical properties such as H^E, η, υ, ρ, and n_D of mixtures comprising glycol ethers and ethers with different groups of hydrocarbon and alcohols compounds led to this work.[4−14] H^E, η, υ, ρ, and n_D for the following mixtures: 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) are measured at p = 0.1 MPa and T = 298.15 and 313.15 K. Δn_D as derivative property are generated by using respectively experimental data of n_D and ρ. Experimental data of ρ of all mixtures are predicted by employing the PC-SAFT EoS.[15,16] Furthermore, the Redlich−Kister equation[17] is used to

Table 1. Chemical Data for the Studied Components

component	formula	molar mass (g/mol)	state mole fraction purity	CAS number
2-(2-methoxyethoxy) ethanol	$C_5H_{12}O_3$	120.15	>0.990[a]	111-77-3
butan-1-ol	$C_4H_{10}O$	74.12	>0.998[a]	71-36-3
butan-2-ol[b]	$C_4H_{10}O$	74.12	>0.990[a]	78-92-2
propan-1-ol	C_3H_8O	60.09	>0.997[a]	71-23-8

[a]Determined by gas chromatography (GC) by the supplier Sigma-Aldrich. [b]Racemic mixture.

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Table 2. Comparison of Experimental Data of Dynamic Viscosities, η, Density, ρ, and Refractive Index, n_D, of 2-(2-Methoxyethoxy)ethanol, Butan-1-ol, Butan-2-ol, and Popan-1-ol with the Corresponding Literature Data at p = 0.1 MPa and T = 298.15 and 313.15 K[a]

	ρ (g/cm^3)		η (mPa·s)		n_D	
T (K)	Exp	Lit	Exp	Lit	Exp	Lit
			2-(2-Methoxyethoxy)ethanol			
298.15	1.0147	1.0154[20]	3.419	3.565[30]	1.4242	1.4250[33]
		1.0164[21]		3.574[31]		1.4245[23]
		1.0150[22]		3.448[24]		1.4233[26]
		1.0167[23]		3.480[32]		1.4233[34]
		1.0164[24]		3.448[24]		1.4245[35]
		1.0153[25]				1.4245[36]
		1.0154[26]				1.4233[37]
		1.0159[27]				1.4245[29]
		1.0164[28]				1.4245[38]
		1.0144[29]				1.4242[39]
313.15	1.0014	1.0020[33]	2.393		1.4183	1.4190[33]
		1.0032[21]				1.4188[35]
		1.0026[27]				
			Butan-1-ol			
298.15	0.8055	0.8060[40]	2.593	2.619[40]	1.3972	1.3972[48]
		0.8059[41]		2.620[44]		1.3972[49]
		0.8057[42]		2.509[42]		1.3972[50]
		0.8057[43]		2.561[43]		1.3967[54]
		0.8060[47]		2.606[47]		1.3993[54]
		0.8057[48]		2.539[48]		1.3974[55]
		0.8056[49]				1.3973[56]
313.15	0.7939	0.7933[40]	1.787	1.786[40]	1.3911	1.3908[54]
		0.7945[41]		1.754[44]		1.3920[55]
		0.7941[42]		1.706[42]		1.3935[63]
		0.7943[43]		1.681[45]		1.3910[63]
		0.7943[45]		1.795[59]		1.3910[66]
		0.7943[47]				
		0.7944[59]				
			Butan-2-ol			
298.15	0.8018	0.8025[48]	3.090	3.093[48]	1.3951	1.3952[48]
		0.8026[49]		3.132[51]		1.3950[49]
		0.8025[56]		3.068[52]		1.3950[50]
		0.8025[56]		2.998[53]		1.3951[56]
		0.8025[57]		2.954[61]		1.3953[56]
		0.8025[61]		3.068[62]		1.3953[61]
		0.8020[52]		2.998[62]		1.3951[66]
		0.8020[62]				
313.15	0.7891	0.7922[58]	1.816	1.801[58]	1.3884	1.3885[61]
		0.7896[59]		1.840[59]		1.3883[63]
		0.7895[59]		1.785[59]		1.3860[63]
		0.7907[60]		1.782[60]		1.3890[66]
		0.7896[61]		1.766[61]		1.3881[66]
		0.7895[63]				
		0.7894[63]				
			Propan-1-ol			
298.15	0.7991	0.7994[40]	1.961	1.981[40]	1.3830	1.3832[54]
		0.7995[41]		1.970[44]		1.3837[54]
		0.7996[42]		1.898[42]		1.3838[55]
		0.7996[47]				1.3836[56]
		0.7996[56]				1.3837[56]
		0.7996[56]				1.3830[66]
		0.7997[57]				
313.15	0.7870	0.7866[40]	1.391	1.381[40]	1.3768	1.3774[54]
		0.7873[41]		1.361[44]		1.3785[55]
		0.7875[42]		1.319[42]		1.3770[66]
		0.7870[46]		1.378[46]		1.3775[66]

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Table 2. continued

	ρ (g/cm^3)		η (mPa·s)		n_D	
T (K)	Exp	Lit	Exp	Lit	Exp	Lit
			Propan-1-ol			
		0.7874[47]		1.379[64]		1.3770[66]
		0.7885[64]		1.379[65]		
		0.7873[65]				

[a]The standard uncertainties u of temperature and pressure are $u(T)$ = 0.04 K and $u(p)$ = 0.001 MPa, respectively. The expanded uncertainties U_c in density and refractive index are $U_c(\rho)$ = 0.0005 g·cm^{-3} and $U_c(n_D)$ = 0.005, respectively, with a 0.95 level of confidence. The relative expanded uncertainty U_r in dynamic viscosity is $U_r(\eta)$ = 2%.

Table 3. Excess Enthalpy, H^E, Uncertainty Budget Using EA-4/02.[68a]

		units	estimate	divisor	$u(x)$ (J·mol^{-1})
$U(Q_{mixture})$	resolution	W	4×10^{-6}	$2\sqrt{3}$	0.8
	repeatability		4×10^{-6}	1	
	nonlinearity		1.2×10^{-4}	1	
$U(\dot{V}_1)$	accuracy	cm^3·s^{-1}	2.5×10^{-5}	2	0.3
	resolution		2.5×10^{-5}	$2\sqrt{3}$	
$U(\dot{V}_2)$	accuracy	cm^3·s^{-1}	2.5×10^{-5}	2	0.3
	resolution		1.7×10^{-5}	$2\sqrt{3}$	
$U(T)$	stability	K	1×10^{-2}	1	0.1
u(H^E)	H^E = 400	J·mol^{-1}		k = 1	0.9
$U(H^E)$		J·mol^{-1}		k = 2	1.8
$U(H^E)$		J·mol^{-1}/J·mol^{-1}		k = 2	5×10^{-3}

[a]$Q_{mixture}$: heat of mixing; $\dot{V}_1$ and $\dot{V}_2$: flows of pure components 1 and 2 driven by isocratic pumps, respectively; T: temperature; H^E: excess enthalpy; x: mole fraction.

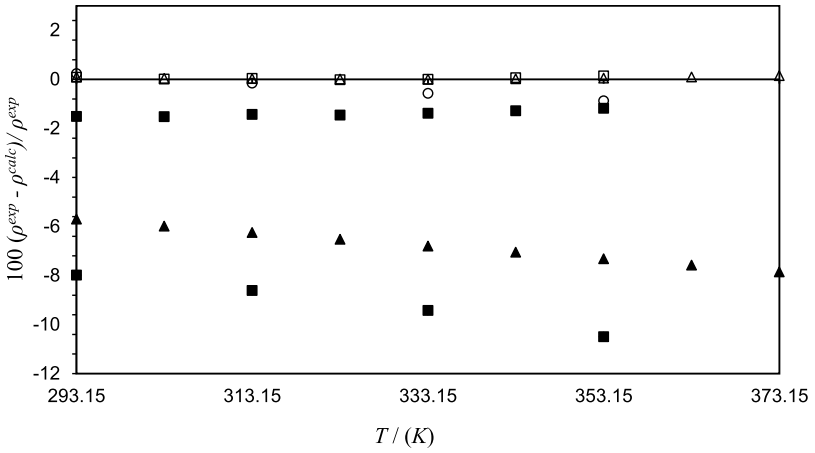

Figure 1. Percentage deviations versus temperature using our estimated PC-SAFT parameters for: (Δ), 1-butanol; (□), 2-butanol; (○), 1-propanol; and using PC-SAFT parameters for: (▲), 1-butanol, Grenner et al.;[72] (■), 2-butanol, Ahmadi et al.;[73] (●), 1-propanol, Grenner et al.[72]

correlate H^E and Δn_D. However, the correlation of measured data of H^E is done using the UNIQUAC[18] and NRTL[19] models.

2. EXPERIMENTAL SECTION

2.1. Chemicals. Chemicals 2-(2-methoxyethoxy)ethanol, butan-1-ol, butan-2-ol, and propan-1-ol are used in this work. Table 1 lists the formula, molar mass, state mole fraction purity, and CAS number of each used chemical. Mixtures comprising 2-(2-methoxyethoxy)ethanol, butan-1-ol, butan-2-ol, and propan-1-ol were generated by mass using an OHAUS balance (precision of 0.0001 g). Table 2 presents a comparison between our reported thermophysical properties (ρ, υ, and n_D) data for each component and data previously reported in the literature.[20−66]

2.2. Apparatus and Procedure. *2.2.2. Excess Enthalpy, H^E.* Measurement of H^E of studied mixtures was generated at the studied temperatures by employing a quasi-isothermal calorimeter. By utilizing the flow rates, molecular weights, and densities of the liquids involved, we determined the various mole fractions (x_i) of the mixtures under investigation. Table 2 provides the densities, ρ, of pure liquids at the measured temperatures. The dependence of H^E on x_i is established by analyzing mixtures of diverse compositions. The H^E is calculated using the following equation: $H^E = \frac{Q_{mixture}}{\dot{n}_{mixture}}$, where $\dot{n}_{mixture}$ is the number of moles per second and $Q_{mixture}$ is the mixing heat. The H^E of binary mixtures is determined by

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Table 4. Excess enthalpy, H^E, Experimental Data of x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2), x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2), and x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2) at p = 0.1 MPa and T = 298.15 and 313.15 K[a]

x	H^E (J·mol^{-1})	x	H^E (J·mol^{-1})	x	H^E (J·mol^{-1})	x	H^E (J·mol^{-1})
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2)[b]							
298.15 K							
0.0496	203.1	0.3005	761.2	0.5504	803.4	0.7998	487.6
0.0994	373.8	0.3496	801.9	0.6000	767.8	0.8490	386.7
0.1495	508.9	0.4000	825.4	0.6494	717.7	0.8994	271.4
0.1998	616.9	0.4502	834.4	0.6999	652.7	0.9491	143.0
0.2501	700.3	0.5004	826.1	0.7501	576.3		
313.15 K							
0.0496	200.9	0.3005	791.9	0.5503	831.8	0.7998	497.3
0.0994	375.6	0.3495	836.5	0.6000	790.5	0.8490	393.2
0.1495	517.5	0.3999	863.6	0.6493	741.4	0.8994	273.1
0.1997	633.5	0.4502	871.4	0.6999	670.7	0.9492	141.5
0.2500	724.9	0.5003	861.9	0.7501	591.0		
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2)[b]							
298.15 K							
0.0498	251.1	0.3001	931.5	0.5499	962.7	0.8005	567.6
0.0999	462.7	0.3505	978.5	0.5995	914.4	0.8496	447.7
0.1500	631.8	0.3995	1003.2	0.6503	850.1	0.8998	311.5
0.2004	761.5	0.4498	1009.7	0.6992	772.7	0.9493	163.7
0.2496	859.9	0.5000	993.8	0.7492	677.0		
313.15 K							
0.0498	214.6	0.3000	881.9	0.5499	920.5	0.8005	537.9
0.0998	412.2	0.3505	931.0	0.5994	872.0	0.8496	423.1
0.1500	574.7	0.3996	956.5	0.6502	809.1	0.8998	293.3
0.2004	705.8	0.4498	964.5	0.6992	732.9	0.9493	153.3
0.2496	805.0	0.5000	950.3	0.7492	644.6		
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2)[b]							
298.15 K							
0.0504	177.0	0.3000	638.9	0.5490	655.5	0.7997	378.9
0.0998	318.4	0.3498	671.6	0.6003	619.7	0.8490	298.4
0.1498	433.2	0.3994	687.5	0.6489	575.1	0.9002	203.8
0.2003	523.5	0.4498	688.6	0.6994	518.3	0.9492	106.1
0.2501	591.4	0.4998	677.8	0.7504	452.0		
313.15 K							
0.0504	180.4	0.2999	673.5	0.5489	688.0	0.7997	393.3
0.0998	328.2	0.3497	706.9	0.6002	648.4	0.8490	308.1
0.1498	450.7	0.3993	725.2	0.6487	601.1	0.9002	209.1
0.2003	547.9	0.4498	726.0	0.6994	540.8	0.9492	108.2
0.2501	620.5	0.4997	713.2	0.7504	470.6		

[a]The standard uncertainties of pressure p, temperature T, and mole fraction x are as follows: $u(p)$ = 0.001 MPa, $u(T)$ = 0.05 K, $u(x)$ = 0.0005. The relative expanded uncertainty (k = 2) is $U_r(H^E)$ = 0.01 for excess enthalpy. [b]x_1: mole fraction of component 1 (2-(2-methoxyethoxy)ethanol).

dividing the mixture's power by the flow rate of moles per second during the mixing process. For binary systems, the two liquids being pumped are pure compounds. The relative expanded uncertainty of H^E is $U_r(H^E)$ = 1% (k = 2), and the standard uncertainty of mole fractions (x_i) of each mixture is $u(x)$ = 0.0005. This experimental technique employed in this paper was deeply validated and described in our previous published work.[67] The uncertainty budget for H^E, as presented in Table 3, was calculated following the guidelines outlined in EA-4/02.[68]

2.2.1. Dynamic and Kinematic Viscosities, (η, υ), Density, (ρ), and Refractive Index, (n_D). Measurement of η, υ, and ρ of pure components and their mixtures was reported at 298.15 and 313.15 K using a Stabinger SVM 3000 viscosimeter. The expanded uncertainties of ρ and η are, respectively, equal to 0.0005 g·cm^{-3} and 0.01 mPa·s (0.95 level of confidence). Furthermore, experimental data of n_D of pure components and their mixtures were also reported at 298.15 and 313.15 K by using an Abbe digital refractometer. The expanded uncertainty of n_D equals 0.005 (0.95 level of confidence). The Abbe digital refractometer (Model Abbemat 300, Anton Paar) is calibrated using air and water; however, the Stabinger SVM 3000 viscosimeter is calibrated using air, water, and decane.

3. ADJUSTMENT OF H^E DATA

The adjustment of H^E data was done using the following Redlich−Kister (R−K) equation[17]

$$H^E = \frac{x\cdot(1-x)\cdot\sum_{i=1}^{n} A_i\cdot(2x-1)^{i-1}}{1 + A_0\cdot(2x-1)} \quad (1)$$

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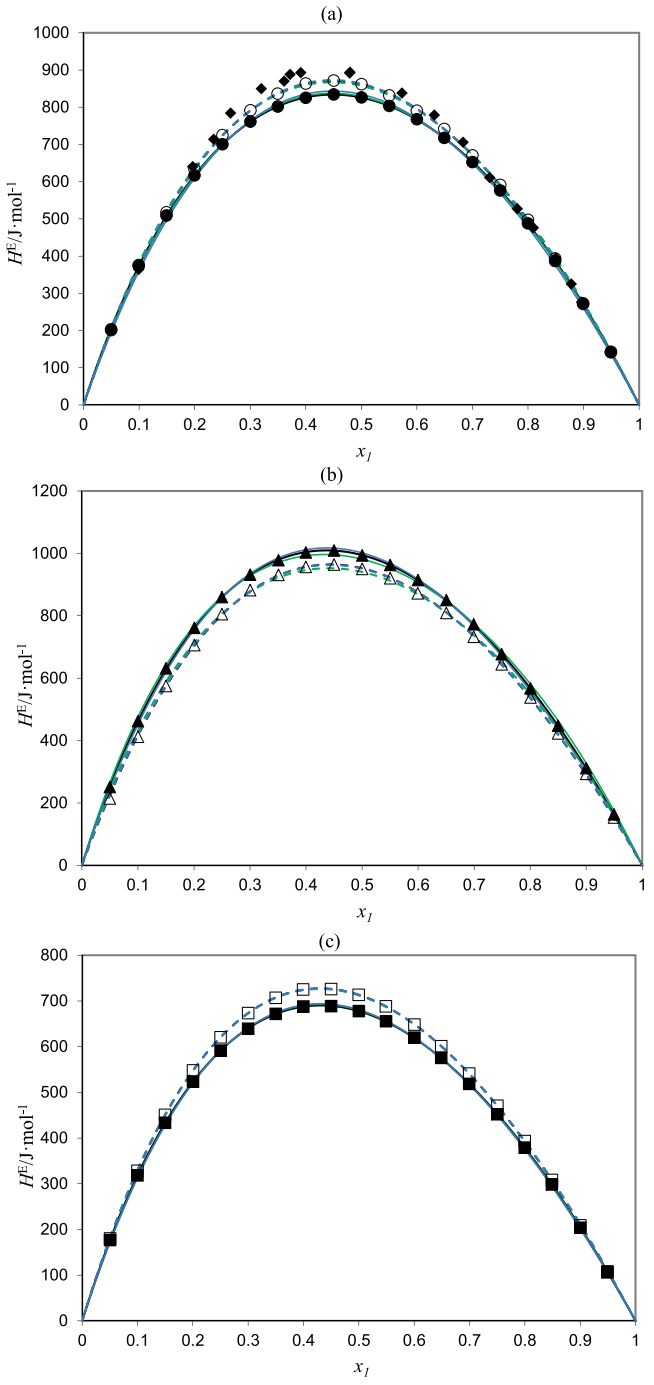

Figure 2. Experimental values of excess enthalpy, H^E, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (●), this work at 298.15 K; (○), this work at 313.15 K; (♦), Cobos et al.;[74] (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 29×8.15 K; (△), this work at 313.15 K; and (c) 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2); (■), this work at 298.15 K; (□), this work at 313.15 K; (—) and (----), calculated values with modified Redlich−Kister equation at 298.15 and 313.15 K, respectively; (green line) and (green dashed line), calculated values with NRTL model at 298.15 and 313.15 K, respectively; (blue line) and (blue dashed line), calculated values with UNIQUAC model at 298.15 and 313.15 K, respectively.

The A_i parameters are determined through the unweighted least-squares method, and the optimal number of A_i was determined through the application of the F-test.[69]

Table 5. Sets of Parameters Needed for the Graphical Representation of Excess Enthalpy, H^E, by Equation 1 for x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2), x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2), and x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2)[a]

	Binary Systems		
	22MEE (1) + 1-But (2)	22MEE (1) + 2-But (2)	22MEE (1) + 1-Pro (2)
		298.15 K	
A_0	0.4150	0.3501	0.3918
A_1	3304.5	3977.9	2711.2
A_2	755.9	457.3	352.7
A_3	123.4	130.1	
MAD (%)	0.1%	0.2%	0.2%
rms ΔH^E (J·mol^{-1})	0.8	1.1	0.8
Max $\lvert\Delta H^E\rvert$ (J·mol^{-1})	1.2	1.2	1.1
Max ($\lvert\Delta H^E\rvert$/H^E)	0.9%	1.0%	1.8%
		313.15 K	
A_0	0.3256	0.2043	0.2754
A_1	3444.0	3809.1	2853.7
A_2	426.2	−74.0	1.482
MAD (%)	0.3%	0.6%	0.2%
rms ΔH^E (J·mol^{-1})	2.2	3.8	0.9
Max $\lvert\Delta H^E\rvert$ (J·mol^{-1})	4.7	4.0	1.2
Max ($\lvert\Delta H^E\rvert$/H^E)	1.6%	4.8%	2.0%

[a]22MEE: 2-(2-methoxyethoxy)ethanol; 1-But: butan-1-ol; 2-But: butan-2-ol; 1-Pro: propan-1-ol.

4. MODELING OF H^E WITH UNIQUAC AND NRTL MODELS

The UNIQUAC[18] and NRTL[19] models are used to predict the H^E data of each mixture in this work. The H^E calculated by the UNIQUAC model is expressed as follows:

$$H^E = \sum_{i=1}^{n} q_i x_i \frac{\sum_{j=1}^{n} \vartheta_j \Delta u_{ji} \tau_{ji}}{\sum_{j=1}^{n} \vartheta_j \tau_{ij}} \tag{2}$$

where x_i is the composition of the mixture; q_i is the molecular surface area; $\vartheta_i = \frac{q_i x_i}{\sum_j q_j x_j}$; $\tau_{ij} = \exp\left[-\frac{u_{ji} - u_{ii}}{RT}\right]$ is the parameter that has same meaning as in the NRTL model; and Δu_{ji} (J mol^{-1}) is the parameter that represents the mixture interaction energy.

The H^E calculated by the NRTL model is generated using the following equation:

$$H^E = -RT \sum_{i=1}^{n} x_i \mu_i \tag{3}$$

where x_i is the composition of the component i.

The μ_i parameters are expressed as follows:

$$\mu_i = \frac{\sum_{k=1}^{p} x_k \tau_{ki} G_{ki} [\alpha(\tau_{ki} - (\sum_{n=1}^{p} x_n \tau_{ni} G_{ni} / \sum_{l=1}^{n} x_l G_{li})) - 1]}{\sum_{l=1}^{p} x_l G_{li}} \tag{4}$$

$$G_{ji} = \exp(-\alpha \tau_{ij}) \tag{5}$$

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Table 6. Sets of Parameters Needed for the Graphical Representation of Excess Enthalpy, H^E, by UNIQUAC and NRTL Models, for x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2), x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2), and x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2)

Binary Systems[a]				
	NRTL		UNIQUAC	
22MEE (1) + 1-But (2)[b]	298.15 K	313.15 K	298.15 K	313.15 K
A_0	0.6461	0.6193	218.7	340.0
A_1	1.3412	1.3279	544.4	390.1
α_{12}	0.30	0.30		
MAD (%)	0.6%	0.7%	1.8%	0.5%
rms ΔH^E (J·mol^{-1})	3.5	3.0	9.1	3.5
Max $\lvert\Delta H^E\rvert$ (J·mol^{-1})	7.4	4.7	15.5	5.7
Max ($\lvert\Delta H^E\rvert/H^E$)	2.0%	3.3%	4.7%	1.6%
	NRTL		UNIQUAC	
22MEE (1) + 2-But (2)[b]	298.15 K	313.15 K	298.15 K	313.15 K
A_0	1.0139	0.7668	198.1	334.3
A_1	1.8692	1.5389	765.0	481.9
α_{12}	0.30	0.30		
MAD (%)	2.0%	2.2%	1.2%	0.6%
rms ΔH^E (J·mol^{-1})	11.0	10.1	7.8	2.5
Max $\lvert\Delta H^E\rvert$ (J·mol^{-1})	16.5	19.1	12.1	6.1
Max ($\lvert\Delta H^E\rvert/H^E$)	7.4%	10.4%	3.2%	5.7%
	NRTL		UNIQUAC	
22MEE (1) + 1-Pro (2)[b]	298.15 K	313.15 K	298.15 K	313.15 K
A_0	0.3422	0.3359	−1.997	99.39
A_1	1.2413	1.2500	661.4	523.8
α_{12}	0.30	0.30		
MAD (%)	0.5%	0.4%	0.8%	0.3%
rms ΔH^E (J·mol^{-1})	2.3	1.2	3.5	0.6
Max $\lvert\Delta H^E\rvert$ (J·mol^{-1})	4.6	3.0	6.1	1.3
Max ($\lvert\Delta H^E\rvert/H^E$)	2.0%	3.2%	2.7%	2.2%

[a]Equivalence between parameters: NRTL $A_0 = \tau_{12}$ and $A_1 = \tau_{21}$; UNIQUAC $A_0 = \Delta u_{12}$; $A_1 = \Delta u_{21}$. [b]22MEE: 2-(2-Methoxyethoxy)ethanol; 1-But: Butan-1-ol; 2-But: Butan-2-ol; 1-Pro: Propan-1-ol.

$$\tau_{ij} = (g_{ij} - g_{ii})/RT \tag{6}$$

where g_{ji} is the interaction energy between each pair of i−j molecules and α is the nonrandomness factor in the mixture.

The following parameters are calculated to have an idea about the quality of the adjusted and correlated data of H^E

$$\text{MAD} = \frac{100}{n_{dat}} \sum_{i=1}^{n_{dat}} \left| \frac{H^E_{exp} - H^E_{calc}}{H^E_{exp}} \right| \tag{7}$$

$$\text{rms} = \left[\frac{\sum_i^{n_{dat}} (H^E_{exp} - H^E_{calc})^2}{n_{dat} - n_{par}} \right]^{1/2} \tag{8}$$

$$\max|\Delta H^E| = \max|H^E_{exp} - H^E_{calc}| \tag{9}$$

$$\max(|\Delta H^E|/H^E) = \max\left(\frac{|H^E_{exp} - H^E_{calc}|}{H^E_{exp}} \right) \tag{10}$$

where H^E_{exp} and H^E_{calc} are the experimental and adjusted data of H^E, respectively, and n_{dat} and n_{par} are the number of experimental data and parameters of the corresponding model, respectively.

5. ADJUSTMENT AND MODELING OF ρ, η, υ, AND N_D AND DERIVATIVE PROPERTIES

5.1. Adjustment. ρ, η, υ, and n_D of each studied mixture are adjusted by using the following mathematical polynomial equation:

$$A(x) = \sum_{i=1}^{N} A_i . x_1^{i-1} \tag{11}$$

where A could be ρ, η, υ, or n_D; x_1 is the composition of component 1; and A_i are parameters generated through the application of the unweighted least-squares method. The determination of the optimal number of A_i was achieved using the F-test.[69]

Δn_D data of each studied mixture are adjusted by using the following R−K equation:

$$\Delta n_D(x) = x_1 . (1 - x_1) . \sum_{i=1}^{N} A_i . (2x_1 - 1)^{i-1} \tag{12}$$

where Δn_D is the deviation in refractive index; x_1 is the composition of component 1; and A_i are parameters that are generated by employing the unweighted least-squares technique.

The deviations of root-mean-square for each adjustment are expressed as follows:

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Table 7. Experimental Data of Dynamic and Kinematic Viscosities, (η, υ), Density, (ρ), and Refractive Index, (n_D), for x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2), x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2), and x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2) at p = 0.1 MPa and T = 298.15 and 313.15 K[a]

x_1	ρ (g/cm^3)	η (mPa·s)	υ (mm^2·s^{-1})	n_D
x_1 2-(2-methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2)[b]				
T = 298.15 K				
0.1005	0.8313	2.37	2.85	1.4002
0.1995	0.8556	2.31	2.70	1.4033
0.3000	0.8790	2.33	2.65	1.4063
0.4010	0.9014	2.40	2.67	1.4092
0.4993	0.9221	2.51	2.72	1.4119
0.5991	0.9422	2.64	2.80	1.4145
0.6995	0.9617	2.80	2.91	1.4171
0.7998	0.9802	2.98	3.04	1.4196
0.9016	0.9981	3.20	3.20	1.4219
T = 313.15 K				
0.1005	0.8194	1.68	2.05	1.3942
0.1995	0.8435	1.66	1.97	1.3973
0.3000	0.8666	1.68	1.94	1.4002
0.4010	0.8888	1.73	1.95	1.4032
0.4993	0.9094	1.81	1.99	1.4059
0.5991	0.9294	1.89	2.04	1.4085
0.6995	0.9487	2.00	2.11	1.4111
0.7998	0.9671	2.12	2.19	1.4136
0.9016	0.9851	2.26	2.29	1.4160
x_1 2-(2-methoxyethoxy)ethanol (1) + (1 − x_1) butan-2-ol (2)[b]				
T = 298.15 K				
0.1012	0.8274	2.62	3.16	1.3982
0.2002	0.8516	2.44	2.87	1.4013
0.2984	0.8748	2.40	2.74	1.4045
0.4007	0.8978	2.44	2.72	1.4076
0.4998	0.9193	2.53	2.75	1.4106
0.6002	0.9401	2.66	2.83	1.4136
0.6988	0.9597	2.81	2.93	1.4164
0.7994	0.9790	2.99	3.05	1.4192
0.9007	0.9975	3.19	3.20	1.4218
T = 313.15 K				
0.1012	0.8147	1.68	2.07	1.3918
0.2002	0.8388	1.64	1.96	1.3950
0.2984	0.8619	1.66	1.92	1.3982
0.4007	0.8849	1.71	1.93	1.4014
0.4998	0.9063	1.79	1.97	1.4045
0.6002	0.9270	1.88	2.03	1.4075
0.6988	0.9466	1.99	2.10	1.4104
0.7994	0.9658	2.11	2.18	1.4132
0.9007	0.9843	2.25	2.28	1.4159
x_1 2-(2-methoxyethoxy)ethanol (1) + (1- x_1) propan-1-ol (2)[b]				
T = 298.15 K				
0.0993	0.8313	1.91	2.30	1.3892
0.2008	0.8606	1.96	2.28	1.3949
0.3004	0.8865	2.06	2.32	1.3999
0.4000	0.9100	2.20	2.41	1.4044
0.4997	0.9314	2.35	2.53	1.4085
0.5997	0.9510	2.53	2.66	1.4122
0.6991	0.9688	2.73	2.82	1.4157
0.7981	0.9852	2.94	2.99	1.4188
0.9011	1.0008	3.18	3.18	1.4218
T = 313.15 K				
0.0993	0.8188	1.38	1.69	1.3832
0.2008	0.8480	1.43	1.69	1.3888
0.3004	0.8737	1.50	1.72	1.3939
0.4000	0.8971	1.60	1.78	1.3983
0.4997	0.9184	1.71	1.86	1.4025
0.5997	0.9379	1.83	1.95	1.4062
0.6991	0.9557	1.95	2.05	1.4097
0.7981	0.9720	2.09	2.15	1.4128
0.9011	0.9876	2.24	2.27	1.4158

[a]The standard uncertainties u of temperature and pressure are $u(T)$ = 0.04 K and $u(p)$ = 0.001 MPa, respectively. The expanded uncertainties U_c in mole fraction, density, and refractive index are $U_c(x)$ = 0.003, $U_c(\rho)$ = 0.0005 g·cm^{-3}, and $U_c(n_D)$ = 0.005, respectively, with a 0.95 level of confidence. The relative expanded uncertainty U_r in dynamic and kinematic viscosities are $U_r(\eta)$ = 2% and $U_r(\upsilon)$ = 2%, respectively. [b]x_1: mole fraction of component 1 (2-(2-methoxyethoxy)ethanol).

$$\sigma(X) = \left[\sum_{i=1}^{N} \frac{(X_{exp} - X_{calc})^2}{(N-p)}\right]^{1/2} \quad (13)$$

where N is the total number of measured data and p is the total number of parameters employed in the R−K equation.

5.2. Modeling of ρ Using PC-SAFT EoS. The PC-SAFT EoS is created by Gross and Sadowski,[15,16] and it is expressed in terms of $\breve{a}^{res}$ (residual Helmholtz energy), as the sum of $\breve{a}^{hc}$, $\breve{a}^{disp}$, and $\breve{a}^{assoc}$:

$$\breve{a}^{res} = \breve{a}^{hc} + \breve{a}^{disp} + \breve{a}^{assoc} \quad (14)$$

where $\breve{a}^{hc}$ is the hard-chain energy contribution; $\breve{a}^{disp}$ is the dispersive energy contribution; and $\breve{a}^{assoc}$ is the association interaction energy.

The nonassociative parameters of PC-SAFT EoS are as follows: σ (segment diameter), m (segment number), and ε/k (segment energy parameter).

Two additional parameters in the case of associative fluids are added to the PC-SAFT EoS: ε^{A_iBI} (the association energy) and $k^{A_iB_i}$ (association volume).

The σ_{ij} and ε_{ij} parameters for the mixture are described by the Berthelot−Lorentz conventional mixing rule

$$\sigma_{ij} = \left(\frac{\sigma_{ii} + \sigma_{jj}}{2}\right) \quad (15)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}(1 - k_{ij}) \quad (16)$$

where k_{ij} is the parameter of binary interaction for correcting the interaction between unequal chain segments. In this work, the binary interaction parameters are assumed to be zero.

The optimization of PC-SAFT EoS parameters was done using the following objective function:

$$\text{Obj. } F = \sum_{i=1}^{M} \left(\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}}\right)^2 \quad (17)$$

where M is the number of experimental data.

The 2B association scheme (two associating sites) was used because of the good representation of density data of all studied mixtures. The association, the shape, and the size of

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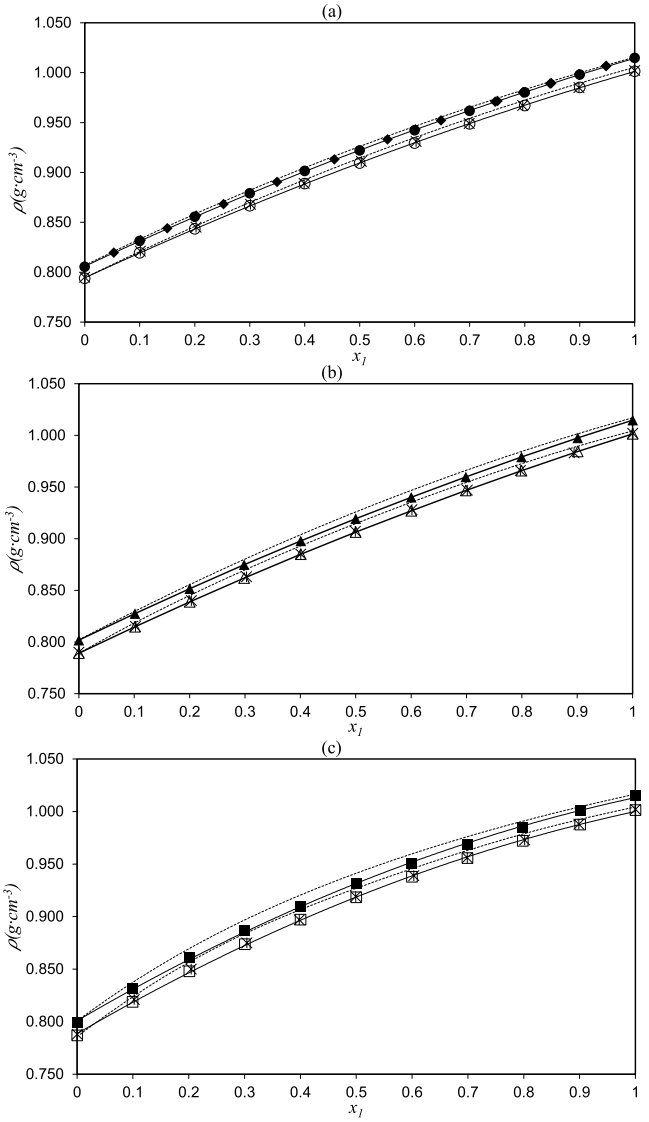

Figure 3. Experimental values of density, ρ, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), at 298.15 K: (●), this work; (♦), Mozo et al.[77] at 313.15 K; (○), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;[78] (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), at 298.15 K; (▲), this work, at 313.15 K; (△), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;[78] and (c) 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2), at 298.15 K; (■), this work, at 313.15 K; (□), this work (Cyrillic capital letter zhe with descender), Belhadj et al.[78] (—), calculated values of density with eq 11; (----), calculated values of density with PC-SAFT equation of state.

the molecules are explicitly taken into account by the PC-SAFT EoS for the reason that it is based on statistical mechanics,[70,71] which is crucial for modeling the density of liquid mixtures.

Figure 1 illustrates the percentage deviations between experimental and calculated densities of pure components (1-butanol, 2-butanol, and 1-propanol) as a function of temperature. These calculations employ our estimated PC-SAFT parameters as well as the parameters reported by Grenner et al.[72] and Ahmadi et al.[73] Our estimated PC-SAFT parameters demonstrate a strong agreement with experimental data for the mentioned pure components, as depicted in Figure 1. The mean absolute deviations (MADs) are as follows: [0.009−.15%], [0.003−0.13%], and [0.23−0.87%] for 1-butanol, 2-butanol, and 1-propanol, respectively, at temperatures of 298.15 and 313.15 K. The PC-SAFT parameters derived from Grenner et al.[72] present a tendency to underestimate the liquid densities of the pure components under investigation. The MADs for 1-butanol and 1-propanol at temperatures of 298.15 and 313.15 K range from 5.70 to 7.85% and 7.98 to 10.49%, respectively. In contrast, for 2-butanol, the PC-SAFT parameters as reported by Ahmadi et al.[73] perform well in predicting the liquid densities of the pure component, showing MADs of 1.18 and 1.52% at temperatures of 298.15 and 313.15 K, respectively. We observed higher deviations in Grenner et al.[72] findings compared to our deviations, and this disparity can be attributed to the fact that Grenner et al.[72] utilized a simplified PC-SAFT approach. In contrast, our parameters exhibit improved predictions when compared to those of Ahmadi et al.,[73] and this can be attributed to our comprehensive fitting methodology. Our parametrization process involved the use of experimental density data exclusively, whereas Ahmadi et al.[73] incorporated both density and vapor pressure data, which could explain the enhanced predictive performance of our parameters in relation to pure component densities. As for 2-(2-methoxyethoxy)-ethanol, no PC-SAFT parameters are available in the literature.

6. RESULTS AND DISCUSSION

H^E, η, υ, ρ, and n_D for the mixtures 2-(2-methoxyethoxy)-ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) are presented at different compositions and at 298.15 and 313.15 K.

6.1. Excess Enthalpy, (H^E). Experimental results of H^E for the following mixtures: 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) are listed in Table 4 and plotted in Figure 2. The A_i parameters to adjust H^E for each studied mixture using eq 1 are listed in Table 5, and Table 6 presents a set of parameters needed for the calculation of H^E by UNIQUAC and NRTL models.

The three studied binary mixtures 2-(2-methoxyethoxy)-ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) show an endothermic behavior ($H^E > 0$) throughout the entire range of x_1 (Figure 2), with a maximum values of H^E of [834.4 J·mol^{-1}, 871.4 J·mol^{-1}], [1009.7 J·mol^{-1}, 964.5 J·mol^{-1}], and [688.6 J·mol^{-1}, 726.0 J·mol^{-1}], respectively, at 298.15 and 313.15 K.

For the 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2) mixture, the best fit of H^E data is obtained with the R−K equation at 298.15 and 313.15 K, with an rms ΔH^E of 0.8 and 2.2 J·mol^{-1}, respectively. The NRTL and UNIQUAC models also exhibit a good correlation, with an rms ΔH^E of [3.5 J·mol^{-1}, 3.0 J·mol^{-1}] and [9.1 J·mol^{-1}, 3.5 J·mol^{-1}], respectively, at 298.15 and 313.15 K. Additionally, in the case of the mixture containing 2-(2-methoxyethoxy)ethanol (1) and butan-2-ol (2), the R−K equation was identified as the most suitable correlation equation for H^E data at 298.15 K, presenting an rms ΔH^E of 1.1 J·mol^{-1}. Conversely, at 313.15 K, the UNIQUAC model demonstrates favorable agreement, resulting in an rms ΔH^E of 2.5 J·mol^{-1}. Finally, in the case of the mixture containing 2-(2-methoxyethoxy)ethanol (1) and propan-1-ol (2), the R−K equation provides the most accurate representation of H^E data at both temperatures, with rms

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Table 8. Sets of Parameters A_i, with Standard Deviations σ, Needed for Adjustment of Dynamic and Kinematic Viscosities, (η, υ), Density, (ρ), and Refractive Index, (n_D), by Employing Equation 11 for the Studied Mixtures at p = 0.1 MPa and T = 298.15 and 313.15 K

	T (K)	A_1	A_2	A_3	A_4	σ
		x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2)[a]				
ρ	298.15	0.80551	0.26338	−0.06502	0.01086	2.6×10^{-8}
	313.15	0.79393	0.25997	−0.06215	0.00975	5.5×10^{-8}
η	298.15	2.5024	−1.0185	1.9816		2.3×10^{-2}
	313.15	1.7403	−0.4546	1.1346		6.4×10^{-3}
υ	298.15	3.0915	−1.9385	2.2839		4.6×10^{-2}
	313.15	2.1828	−1.0881	1.3348		1.4×10^{-2}
n_D	298.15	1.3972	0.0315	−0.0040	−0.0004	1.1×10^{-8}
	313.15	1.3911	0.0321	−0.0051	0.0003	1.2×10^{-8}
		x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2)[a]				
ρ	298.15	0.80176	0.25879	−0.04891	0.00309	2.9×10^{-8}
	313.15	0.78908	0.25822	−0.04917	0.00331	2.9×10^{-8}
η	298.15	2.9095	−2.2585	2.8605		9.2×10^{-2}
	313.15	1.7574	−0.6027	1.2717		1.0×10^{-2}
υ	298.15	3.6090	−3.5033	3.3904		1.7×10^{-1}
	313.15	2.2176	−1.2756	1.4956		2.1×10^{-2}
n_D	298.15	1.3951	0.0313	0.0014	−0.0035	7.7×10^{-9}
	313.15	1.3884	0.0338	−0.0023	−0.0015	8.4×10^{-9}
		x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2)[a]				
ρ	298.15	0.79929	0.33572	−0.16419	0.04401	2.2×10^{-7}
	313.15	0.78716	0.33254	−0.16046	0.04230	1.8×10^{-7}
η	298.15	1.9063	0.2057	1.3382		9.1×10^{-3}
	313.15	1.3605	0.3088	0.7422		2.9×10^{-3}
υ	298.15	2.3741	−0.4884	1.5289		1.9×10^{-2}
	313.15	1.7220	−0.1859	0.8805		6.4×10^{-3}
n_D	298.15	1.3831	0.0648	−0.0318	0.0082	3.0×10^{-8}
	313.15	1.3769	0.0655	−0.0330	0.0089	5.1×10^{-8}

[a] x_1: mole fraction of component 1 (2-(2-methoxyethoxy)ethanol).

ΔH^E values of 0.8 and 0.9 J·mol^{-1}, respectively. Furthermore, the NRTL and UNIQUAC models exhibit also favorable agreements at both temperatures.

Our experimental H^E data for the 2-(2-methoxyethoxy)-ethanol (1) and butan-1-ol (2) mixture were compared to data reported by Cobos et al.[74] The comparison, as illustrated in Figure 2a, reveals close agreement between our experimental data and the referenced data, with a MAD of only 4.4%. Importantly, at a temperature of 313.15 K, we found no reference data available in the literature for a similar comparative analysis. Moreover, no reference data were found in the literature for the mixtures of 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2) and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) at the two temperatures under investigation.

The understanding of enthalpic effects (H^E) plays a crucial role in grasping the nonideal characteristics of the final mixture solution. This particular concept relates to the impact of variations in shape and size among different molecules, as well as the diverse interactions between them, which can result in either an increase or a decrease in H^E values.[75] Within this context, the mixtures 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2) show an endothermic behavior at the studied temperatures and throughout the entire range of x_1. The observed behavior in these three mixtures was expected, as it can be attributed to the disruption of intermolecular hydrogen bonds during the combination of 2-(2-methoxyethoxy)ethanol, a glycol ether, with various alcohols, including butan-1-ol, butan-2-ol, and propan-1-ol.

The comparison among mixtures of 2-(2-methoxyethoxy)-ethanol (1) with butan-1-ol (2), butan-2-ol (2), and propan-1-ol (2) reveals that, for a given 2-(2-methoxyethoxy)ethanol, the H^E values at both temperatures (298.15 and 313.15 K) followed the order: propan-1-ol < butan-1-ol < butan-2-ol. This comparison also reveals a slight variation in H^E values between 298.15 and 313.15 K. Specifically, for the mixture of 2-(2-methoxyethoxy)ethanol (1) with butan-1-ol (2), there is a difference of 37 J·mol^{-1} between the two temperatures. Similarly, the mixture of 2-(2-methoxyethoxy)ethanol (1) with propan-1-ol (2) shows a difference of 37.4 J·mol^{-1}, and finally the mixture of 2-(2-methoxyethoxy)ethanol (1) with butan-2-ol (2) exhibits a difference of 45.2 J·mol^{-1}. The minimal variation in H^E values between the temperatures examined for the mixtures can be attributed to the similarity in the surface properties of butan-1-ol, butan-2-ol, and propan-1-ol. The maximum H^E values for the mixtures of 2-(2-methoxyethoxy)ethanol (1) with butan-1-ol (2), butan-2-ol (2), and propan-1-ol (2) were in the ranges of [834.4−871.4 J·mol^{-1}], [1009.7−964.5 J·mol^{-1}], and [688.6−726.0 J·mol^{-1}] at 298.15 and 313.15 K, respectively.

The H^E versus x_1 plots exhibit a nearly symmetrical pattern for all studied mixtures: 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propa-1-ol (2). The H^E of these mixtures may be influenced by different factors such as (i) liberation of heat as a result of possible

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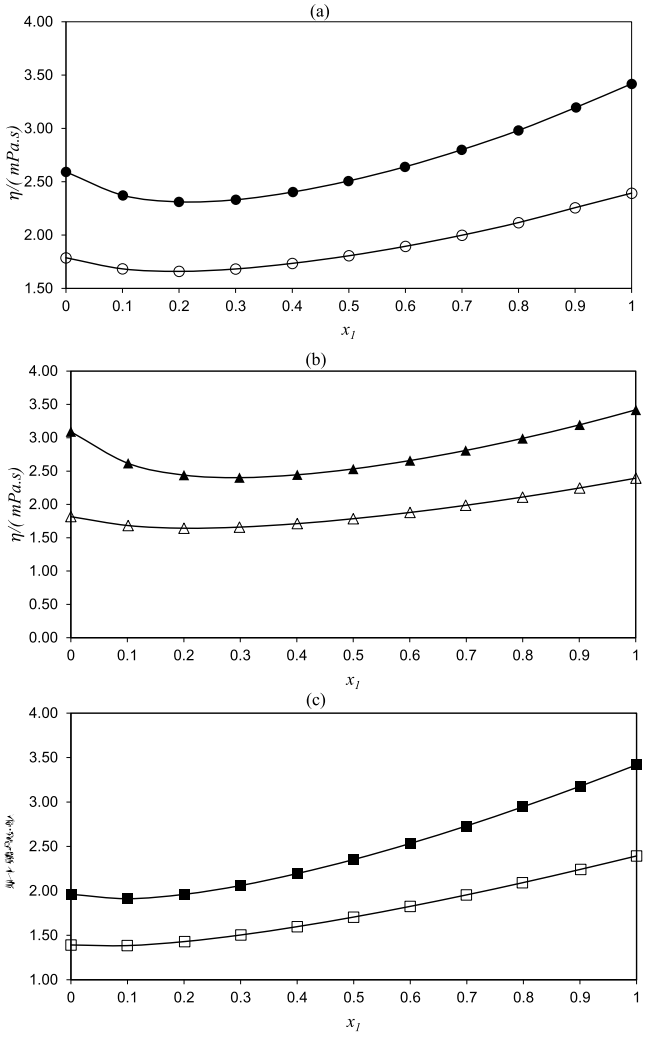

Figure 4. Experimental values of dynamic viscosity, η, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (●), this work at 298.15 K; (○), this work at 313.15 K; (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 298.15 K; (△), this work at 313.15 K; and (c) 2-(2-methoxyethoxy)-ethanol (1) + propan-1-ol (2); (■), this work at 298.15 K; (□), this work at 313.15 K. (—), calculated values of dynamic viscosity with eq 11.

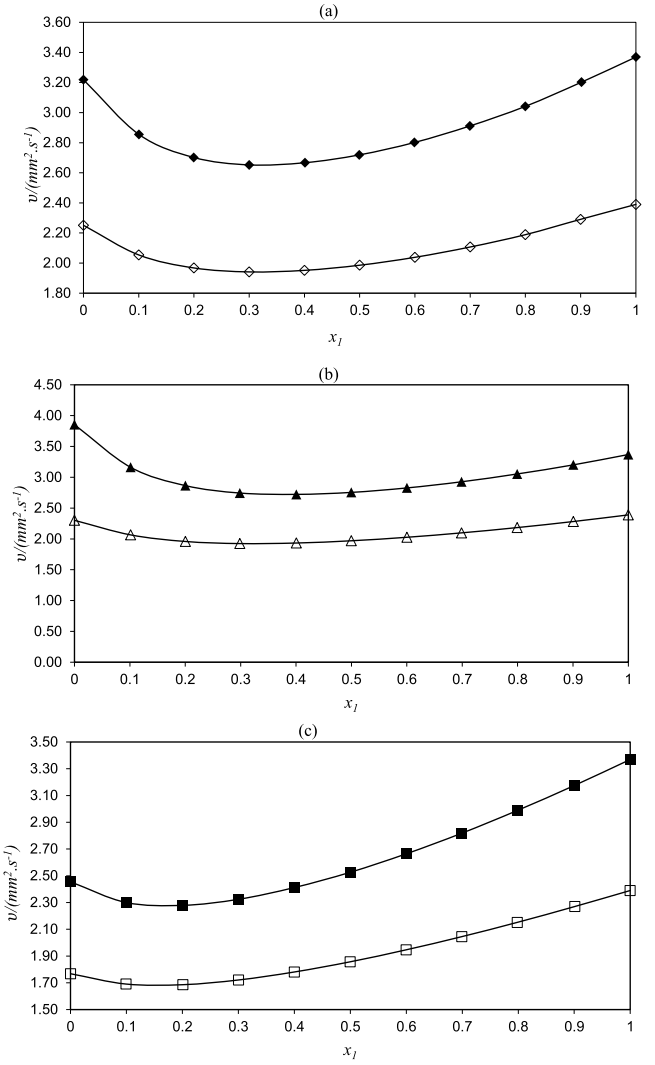

Figure 5. Experimental values of kinematic viscosity, υ, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (♦), this work at 298.15 K; (◊), this work at 313.15 K; (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 298.15 K; (△), this work at 313.15 K; and (c) 2-(2-methoxyethoxy)-ethanol (1) + propan-1-ol (2); (■), this work at 298.15 K; (□), this work at 313.15 K. (—), calculated values of kinematic viscosity with eq 11.

hydrogen bonding interaction between the ether group of the alkoxyethanol (2-(2-methoxyethoxy)ethanol) and the hydroxyl function of the alcohol (butan-1-ol, butan-2-ol or propa-1-ol) and (ii) absorption of heat due to depolymerization of self-associated alcohols or 2-(2-methoxyethoxy)ethanol as a glycol ether.[76]

6.2. Dynamic and Kinematic Viscosities, (η, υ), Density, ρ, and Refractive Index, n_D. Experimental results of η, υ, ρ, and n_D are reported at 298.15 and 313.15 K and 0.1 MPa to explain and to understand the nature of different molecular interactions between distinct studied mixtures: 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), + butan-2-ol (2), and + propa-1-ol (2). These thermophysical properties of each studied mixture are presented in Table 7 and plotted in Figures 3−6. The A_i parameters used to adjust ρ, η, υ, and n_D of each studied mixture using eq 11 are listed in Table 8. Figures 3 and 6 indicate, respectively, that the values of ρ and n_D increase with an increase in x_1 and decrease with an increase in temperature. While Figures 4 and 5 show that η and υ values decrease as the temperature increases from 298.15 to 313.15 K, they also decrease vs x_1, and until they have reached certain fractions, the viscosities increase with the augmentation of x_1. We compared our experimental density data at 298.15 K for the mixture of 2-(2-methoxyethoxy)ethanol (1) and butan-1-ol (2) to the data reported by Mozo et al.[77] The comparison (Figure 3a) revealed a strong agreement with a MAD of only 0.05%. Similarly, at 313.15 K, we compared our experimental density and refractive index data for three studied mixtures: 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2), and 2-(2-methoxyethoxy)ethanol (1) + propa-1-ol (2) to the data reported by Belhadj et al.[78] In all cases, the comparison showed excellent agreement, with MADs of 0.09, 0.05, and 0.08% for density (Figure 3) and 0.04, 0.03, and 0.03% for refractive index (Figure 6), respectively.

The PC-SAFT EoS parameters of each studied component are listed in Table 9, and as shown in Figure 3, the associated

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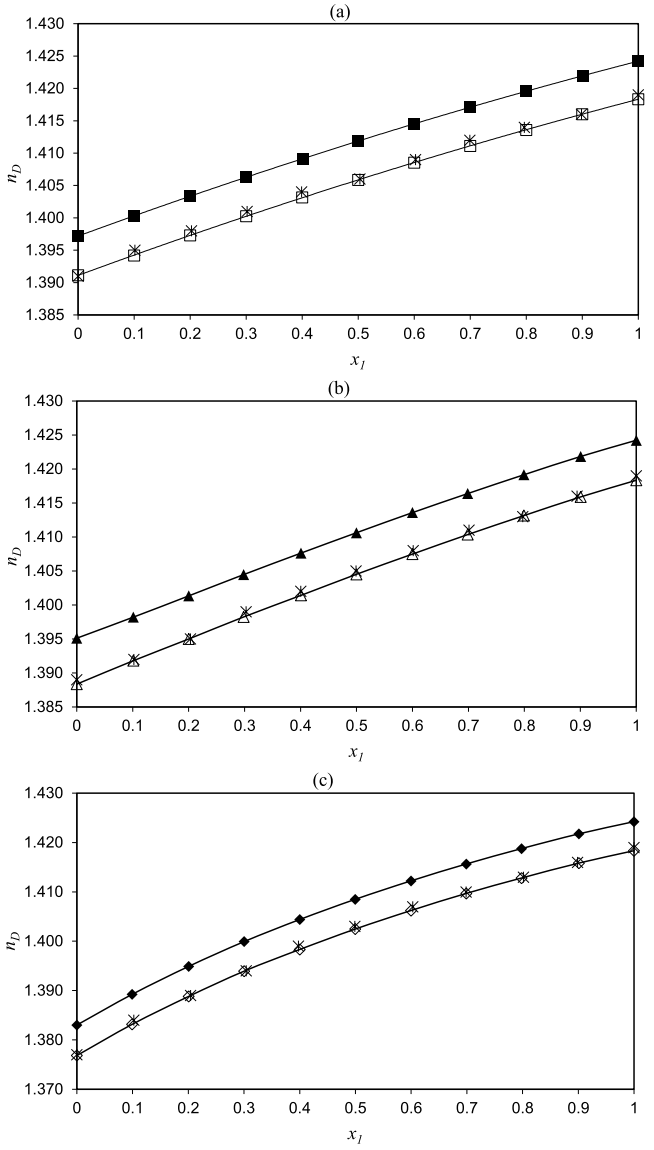

Figure 6. Experimental values of refractive index, n_D, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), at 298.15 K; (■), this work, at 313.15 K; (□), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;[78] (b) 2-(2-methoxyethoxy)-ethanol (1) + butan-2-ol (2), at 298.15 K: (▲), this work, at 313.15 K; (△), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;[78] and (c) 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2), at 298.15 K; (♦), this work, at 313.15 K; (◊), this work (Cyrillic capital letter zhe with descender), Belhadj et al.[78] (—), calculated values of refractive index with eq 11.

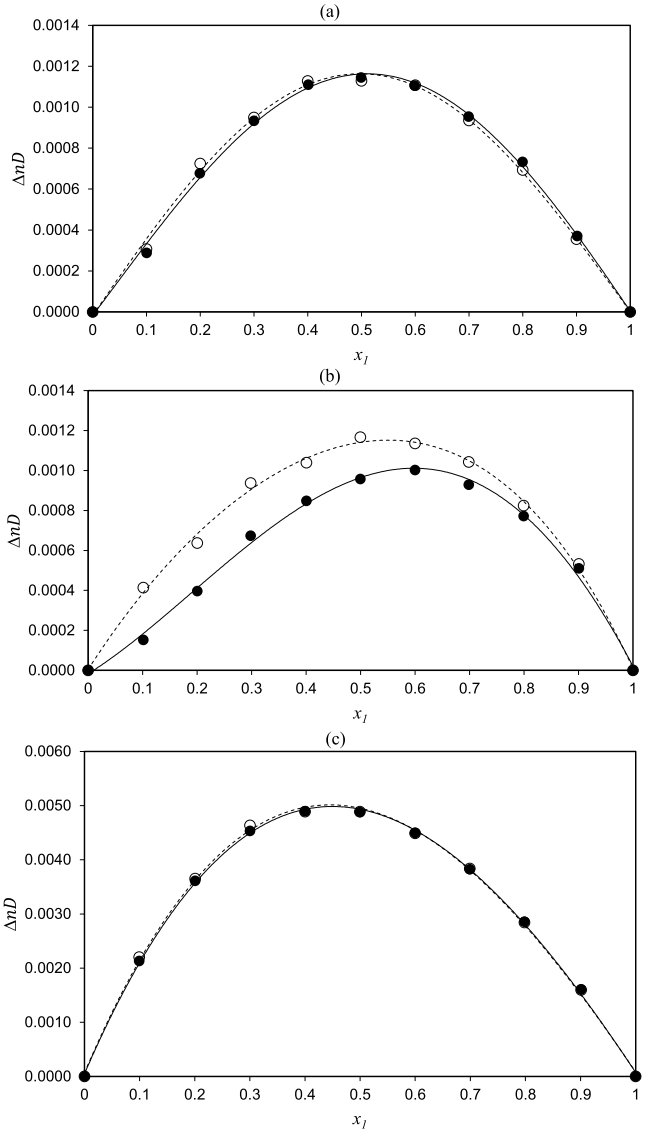

Figure 7. Calculated values of deviations in refractive index, Δn_D, as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); and (c) 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2). At temperatures: (●), 298.15 K and (○), 313.15 K. Calculated values of Δn_D with eq 12: (--) at 298.15 K and (----) at 313.15 K.

densities are also represented using the PC-SAFT EoS. The results show that all studied mixtures accord well with experimental data. In addition, the *MAD* values for the studied mixtures 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), + butan-2-ol (2), and + propa-1-ol (2), at 298.15 and 313.15 K are, respectively, within [0.03−0.72%], [0.06−0.77%], and [0.18−1.16%]. There is a good agreement between the predicted values of density and the experimental data when compared,[70,71] and this is due to the effect that PC-SAFT EoS clearly takes into account the association, the shape, and the size of the molecules, which is crucial for modeling the studied mixtures.

Table 9. PC-SAFT EoS Parameters for 2-(2-Methoxyethoxy)ethanol, Butan-1-ol, Butan-2-ol, and Propan-1-ol

compound	m	σ [A]	ε/k [K]	ε^{HB}/k [K]	K^{HB} [K]	MAD % (ρ^{Liq})
2-(2-methoxyethoxy) ethanol	5.82427	3.05987	245.707	0.105827	3767.82	0.04
butan-1-ol	4.38072	3.04936	218.502	0.040269	2246.18	0.03
butan-2-ol	3.68544	3.21794	213.009	0.031205	2085.52	0.04
propan-1-ol	2.60020	3.37781	275.455	0.010010	1040.45	0.05

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Table 10. Sets of Parameters A_i, with Standard Deviations σ, Using for Adjustment of Deviations in Refractive Index, Δn_D, by Employing the Redlich-Kister Equation for the Studied Binary Mixtures at 298.15 and 313.15 K and at 0.1 MPa

	T (K)	A_1	A_2	A_3	σ
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-1-ol (2)[a]					
Δn_D	298.15	0.00465	0.00027	−0.00108	4.8×10^{-9}
	313.15	0.00465	−0.00003	−0.00102	6.4×10^{-9}
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Butan-2-ol (2)[a]					
Δn_D	298.15	0.00386	0.00191	−0.00039	7.3×10^{-9}
	313.15	0.00456	0.00084	0.00059	6.6×10^{-9}
x_1 2-(2-Methoxyethoxy)ethanol (1) + (1 − x_1) Propan-1-ol (2)[a]					
Δn_D	298.15	0.01950	−0.00400	0.00202	3.7×10^{-9}
	313.15	0.01953	−0.00440	0.00247	1.2×10^{-8}

[a] x_1: mole fraction of component 1 (2-(2-methoxyethoxy)ethanol).

6.3. Deviation in Refractive Index, (Δn_D). Δn_D is calculated for the mixtures of 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), + butan-2-ol (2), and + propa-1-ol (2) by employing the following equation:

$$\Delta n_D = n_D - \sum_{i+1}^{N} x_i n_{Di} \tag{18}$$

where n_i is the component i refractive index and n_D is the mixture refractive index.

Figure 7 presents the calculated Δn_D for the mixtures of 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), + butan-2-ol (2), and + propa-1-ol (2), at 298.15 and 313.15 K, and over the entire range of x_1. The A_i parameters used to adjust the Δn_D of each studied mixture using eq 12 are listed in Table 10. The calculated values of Δn_D are all positive for all of the studied mixtures. While the chain length of the alkanol decreases, the change in Δn_D becomes more positive. It is also true that Δn_D values of these mixtures changed slightly more positively at higher temperatures compared to the change observed between 298.15 and 313.15 K.

7. CONCLUSIONS

Experimental data of H^E, η, υ, ρ, and n_D are reported for mixtures containing 2-(2-methoxyethoxy)ethanol (1) with 1-butanol or 2-butanol or 1-propanol at T = 298.15 and 313.15 K and over a wide range of composition. From the presented experimental results, the derivative property as Δn_D was also determined. The PC-SAFT EoS was used to predict the ρ values for all studied mixtures, and it showed good agreement with the reported experimental results of ρ. The impacts of intermolecular interaction are examined for each studied mixture.

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Notes

The authors declare no competing financial interest.

LIST OF SYMBOLS

H^E:excess enthalpy; η:dynamic viscosity; υ:kinematic viscosity; ρ:density; n_D:refractive index; Δn_D:deviations in refractive index; p:pressure; T:temperature; i:constituent identification; x_i:mole fraction of component i; EoS:equation of state; R−K:Redlich−Kister; MAD:absolute relative mean deviation; max|ΔH^E|:absolute difference maximum; max(|ΔH^E|/H^E):maximum relative deviation; rms:root-mean-square deviation

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