

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

Mohamed Lifi,* Ilham Abala, Raúl Briones-Llorente, Natalia Muñoz-Rujas, Fernando Aguilar, and Fatima Ezzahrae M'hamdi Alaoui

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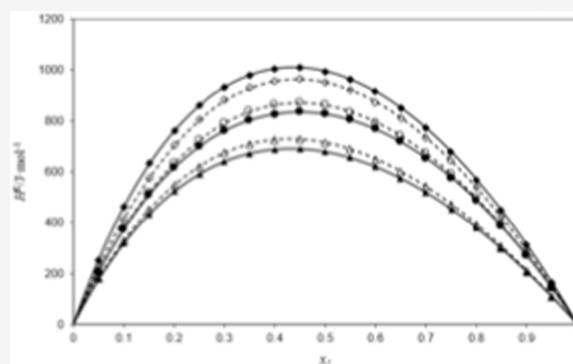
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ABSTRACT: Excess enthalpy (H^E), dynamic and kinematic viscosities (η , ν), density (ρ), and refractive index (n_D) of mixtures comprising 2-(2-methoxyethoxy)ethanol, butan-1-ol, butan-2-ol, and propan-1-ol are presented at $p = 0.1$ MPa and at $T = 298.15$ 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 , ν , 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 , ν , 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 equation¹⁷ 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 ₅ H ₁₂ O ₃ | 120.15 | >0.990 ^a | 111-77-3 |
| butan-1-ol | C ₄ H ₁₀ O | 74.12 | >0.998 ^a | 71-36-3 |
| butan-2-ol ^b | C ₄ H ₁₀ O | 74.12 | >0.990 ^a | 78-92-2 |
| propan-1-ol | C ₃ H ₈ O | 60.09 | >0.997 ^a | 71-23-8 |

^aDetermined by gas chromatography (GC) by the supplier Sigma-Aldrich. ^bRacemic mixture.

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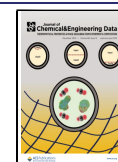


Table 2. Comparison of Experimental Data of Dynamic Viscosities, η , Density, ρ , and Refractive Index, n_D , of 2-(2-Methoxyethoxy)ethanol, Butan-1-ol, Butan-2-ol, and Popan-1-ol with the Corresponding Literature Data at $p = 0.1$ MPa and $T = 298.15$ and 313.15 K^a

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

Table 2. continued

| T (K) | ρ (g/cm ³) | | η (mPa·s) | | n_D | |
|-------|-----------------------------|----------------------|----------------|---------------------|-------|----------------------|
| | 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 | | | | |

^aThe 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) |
|-------------------------|---------------|--|----------------------|-------------|-------------------------------|
| $U(Q_{\text{mixture}})$ | 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.

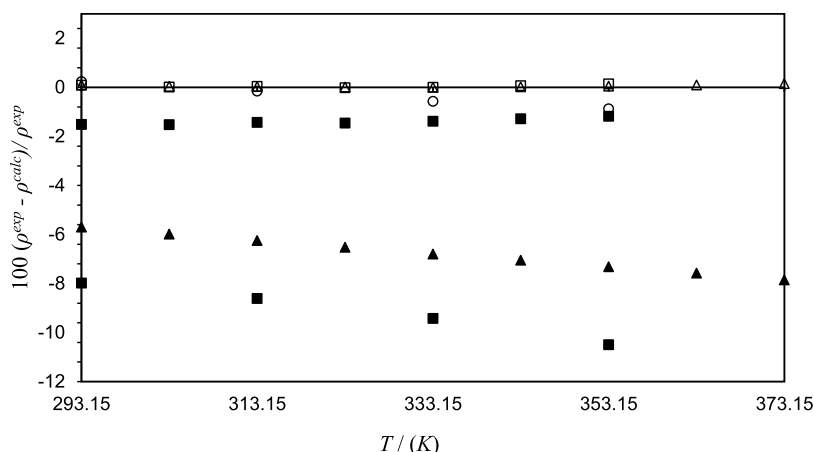


Figure 1. Percentage deviations versus temperature using our estimated PC-SAFT parameters for: (Δ), 1-butanol; (\square), 2-butanol; (\circ), 1-propanol; and using PC-SAFT parameters for: (\blacktriangle), 1-butanol, Grenner et al.,⁷² (\blacksquare), 2-butanol, Ahmadi et al.,⁷³ (\bullet), 1-propanol, Grenner et al.⁷²

correlate H^E and Δn_D . However, the correlation of measured data of H^E is done using the UNIQUAC¹⁸ and NRTL¹⁹ 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 , v , 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: $H^E = \frac{Q_{\text{mixture}}}{\dot{n}_{\text{mixture}}}$, 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

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 | | |

^aThe 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 , ν), Density, (ρ), and Refractive Index, (n_D). Measurement of η , ν , 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) equation¹⁷

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

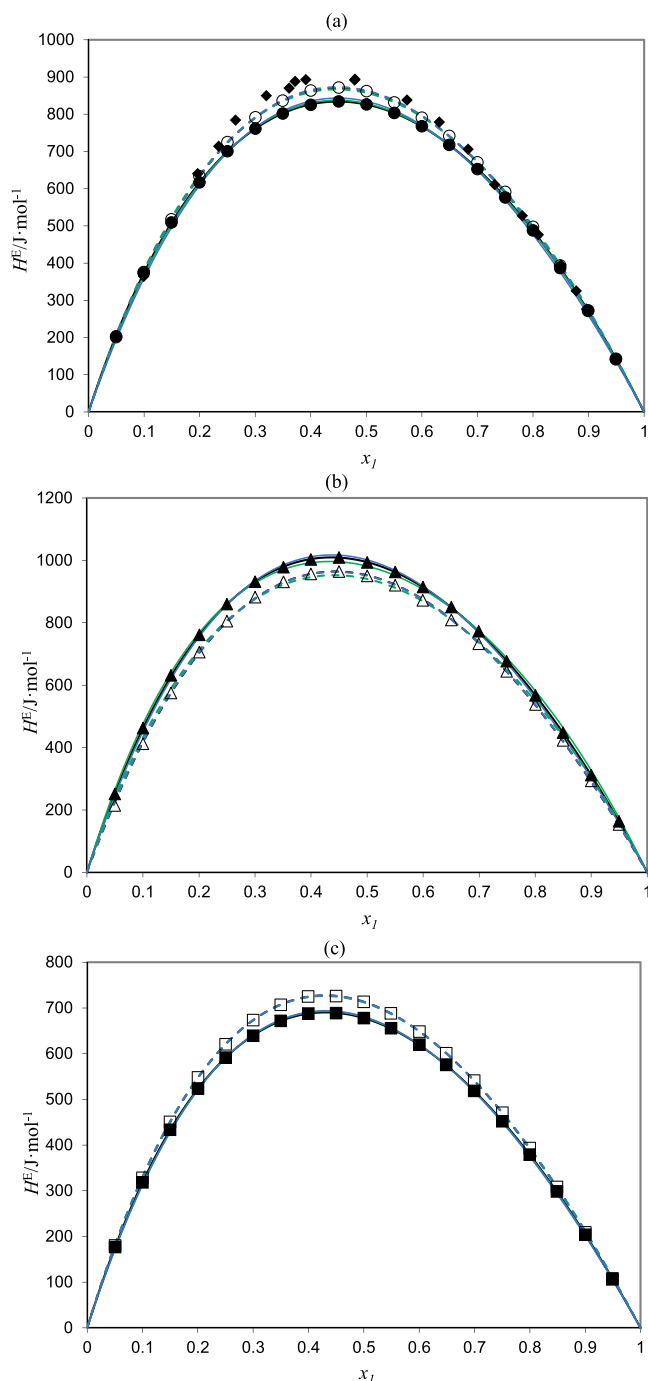


Figure 2. Experimental values of excess enthalpy, H^E , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (●), this work at 298.15 K; (○), this work at 313.15 K; (◆), Cobos et al.;⁷⁴ (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 298.15 K; (△), this 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; (—) 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 $ \Delta H^E $ (J·mol ⁻¹) | 1.2 | 1.2 | 1.1 |
| Max $(\Delta H^E /$ $H^E)$ | 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 $ \Delta H^E $ (J·mol ⁻¹) | 4.7 | 4.0 | 1.2 |
| Max $(\Delta H^E /$ $H^E)$ | 1.6% | 4.8% | 2.0% |

^a22MEE: 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 UNIQUAC¹⁸ and NRTL¹⁹ 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:

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

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:

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

where x_i is the composition of the component i .

The μ_i parameters are expressed as follows:

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

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

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 | | | | |
|---|----------|----------|----------|----------|
| 22MEE (1) + 1-But (2) ^b | NRTL | | UNIQUAC | |
| | 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 $ \Delta H^E $ (J·mol ⁻¹) | 7.4 | 4.7 | 15.5 | 5.7 |
| Max ($ \Delta H^E /H^E$) | 2.0% | 3.3% | 4.7% | 1.6% |
| 22MEE (1) + 2-But (2) ^b | NRTL | | UNIQUAC | |
| | 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 $ \Delta H^E $ (J·mol ⁻¹) | 16.5 | 19.1 | 12.1 | 6.1 |
| Max ($ \Delta H^E /H^E$) | 7.4% | 10.4% | 3.2% | 5.7% |
| 22MEE (1) + 1-Pro (2) ^b | NRTL | | UNIQUAC | |
| | 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 $ \Delta H^E $ (J·mol ⁻¹) | 4.6 | 3.0 | 6.1 | 1.3 |
| Max ($ \Delta H^E /H^E$) | 2.0% | 3.2% | 2.7% | 2.2% |

^aEquivalence between parameters: NRTL $A_0 = \tau_{12}$ and $A_1 = \tau_{21}$; UNIQUAC $A_0 = \Delta u_{12}$; $A_1 = \Delta u_{21}$. ^b22MEE: 2-(2-Methoxyethoxy)ethanol; 1-But: Butan-1-ol; 2-But: Butan-2-ol; 1-Pro: Propan-1-ol.

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

where g_{ij} 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

$$\text{MAD} = \frac{100}{n_{\text{dat}}} \sum_{i=1}^{n_{\text{dat}}} \left| \frac{H_{\text{exp}}^E - H_{\text{calc}}^E}{H_{\text{exp}}^E} \right| \quad (7)$$

$$\text{rms} = \left[\frac{\sum_{i=1}^{n_{\text{dat}}} (H_{\text{exp}}^E - H_{\text{calc}}^E)^2}{n_{\text{dat}} - n_{\text{par}}} \right]^{1/2} \quad (8)$$

$$\text{max}|\Delta H^E| = \text{max}|H_{\text{exp}}^E - H_{\text{calc}}^E| \quad (9)$$

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

where H_{exp}^E and H_{calc}^E 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 , v , AND n_D AND DERIVATIVE PROPERTIES

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

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

where A could be ρ , η , v , 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:

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

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:

Table 7. Experimental Data of Dynamic and Kinematic Viscosities, (η , ν), 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) | ν (mm ² ·s ⁻¹) | n_D | x_1 | ρ (g/cm ³) | η (mPa·s) | ν (mm ² ·s ⁻¹) | n_D |
|---|-----------------------------|----------------|---|--------|--|-----------------------------|----------------|---|--------|
| x_1 2-(2-methoxyethoxy)ethanol (1) + (1 - x_1) Butan-1-ol (2) ^b | | | | | x_1 2-(2-methoxyethoxy)ethanol (1) + (1 - x_1) propan-1-ol (2) ^b | | | | |
| $T = 298.15$ K | | | | | $T = 298.15$ K | | | | |
| 0.1005 | 0.8313 | 2.37 | 2.85 | 1.4002 | 0.4007 | 0.8849 | 1.71 | 1.93 | 1.4014 |
| 0.1995 | 0.8556 | 2.31 | 2.70 | 1.4033 | 0.4998 | 0.9063 | 1.79 | 1.97 | 1.4045 |
| 0.3000 | 0.8790 | 2.33 | 2.65 | 1.4063 | 0.6002 | 0.9270 | 1.88 | 2.03 | 1.4075 |
| 0.4010 | 0.9014 | 2.40 | 2.67 | 1.4092 | 0.6988 | 0.9466 | 1.99 | 2.10 | 1.4104 |
| 0.4993 | 0.9221 | 2.51 | 2.72 | 1.4119 | 0.7994 | 0.9658 | 2.11 | 2.18 | 1.4132 |
| 0.5991 | 0.9422 | 2.64 | 2.80 | 1.4145 | 0.9007 | 0.9843 | 2.25 | 2.28 | 1.4159 |
| 0.6995 | 0.9617 | 2.80 | 2.91 | 1.4171 | $T = 313.15$ K | | | | |
| 0.7998 | 0.9802 | 2.98 | 3.04 | 1.4196 | 0.0993 | 0.8313 | 1.91 | 2.30 | 1.3892 |
| 0.9016 | 0.9981 | 3.20 | 3.20 | 1.4219 | 0.2008 | 0.8606 | 1.96 | 2.28 | 1.3949 |
| $T = 313.15$ K | | | | | 0.3004 | 0.8865 | 2.06 | 2.32 | 1.3999 |
| 0.1005 | 0.8194 | 1.68 | 2.05 | 1.3942 | 0.4000 | 0.9100 | 2.20 | 2.41 | 1.4044 |
| 0.1995 | 0.8435 | 1.66 | 1.97 | 1.3973 | 0.4997 | 0.9314 | 2.35 | 2.53 | 1.4085 |
| 0.3000 | 0.8666 | 1.68 | 1.94 | 1.4002 | 0.5997 | 0.9510 | 2.53 | 2.66 | 1.4122 |
| 0.4010 | 0.8888 | 1.73 | 1.95 | 1.4032 | 0.6991 | 0.9688 | 2.73 | 2.82 | 1.4157 |
| 0.4993 | 0.9094 | 1.81 | 1.99 | 1.4059 | 0.7981 | 0.9852 | 2.94 | 2.99 | 1.4188 |
| 0.5991 | 0.9294 | 1.89 | 2.04 | 1.4085 | 0.9011 | 1.0008 | 3.18 | 3.18 | 1.4218 |
| 0.6995 | 0.9487 | 2.00 | 2.11 | 1.4111 | $T = 313.15$ K | | | | |
| 0.7998 | 0.9671 | 2.12 | 2.19 | 1.4136 | 0.0993 | 0.8188 | 1.38 | 1.69 | 1.3832 |
| 0.9016 | 0.9851 | 2.26 | 2.29 | 1.4160 | 0.2008 | 0.8480 | 1.43 | 1.69 | 1.3888 |
| x_1 2-(2-methoxyethoxy)ethanol (1) + (1 - x_1) butan-2-ol (2) ^b | | | | | 0.3004 | 0.8737 | 1.50 | 1.72 | 1.3939 |
| $T = 298.15$ K | | | | | 0.4000 | 0.8971 | 1.60 | 1.78 | 1.3983 |
| 0.1012 | 0.8274 | 2.62 | 3.16 | 1.3982 | 0.4997 | 0.9184 | 1.71 | 1.86 | 1.4025 |
| 0.2002 | 0.8516 | 2.44 | 2.87 | 1.4013 | 0.5997 | 0.9379 | 1.83 | 1.95 | 1.4062 |
| 0.2984 | 0.8748 | 2.40 | 2.74 | 1.4045 | 0.6991 | 0.9557 | 1.95 | 2.05 | 1.4097 |
| 0.4007 | 0.8978 | 2.44 | 2.72 | 1.4076 | 0.7981 | 0.9720 | 2.09 | 2.15 | 1.4128 |
| 0.4998 | 0.9193 | 2.53 | 2.75 | 1.4106 | 0.9011 | 0.9876 | 2.24 | 2.27 | 1.4158 |
| 0.6002 | 0.9401 | 2.66 | 2.83 | 1.4136 | $T = 313.15$ K | | | | |
| 0.6988 | 0.9597 | 2.81 | 2.93 | 1.4164 | 0.1012 | 0.8147 | 1.68 | 2.07 | 1.3918 |
| 0.7994 | 0.9790 | 2.99 | 3.05 | 1.4192 | 0.2002 | 0.8388 | 1.64 | 1.96 | 1.3950 |
| 0.9007 | 0.9975 | 3.19 | 3.20 | 1.4218 | 0.2984 | 0.8619 | 1.66 | 1.92 | 1.3982 |

^aThe 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 $U_r(\nu) = 2\%$, respectively. ^b x_1 : mole fraction of component 1 (2-(2-methoxyethoxy)ethanol).

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

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 \tilde{a}^{res} (residual Helmholtz energy), as the sum of \tilde{a}^{hc} , \tilde{a}^{disp} , and \tilde{a}^{assoc} :

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

where \tilde{a}^{hc} is the hard-chain energy contribution; \tilde{a}^{disp} is the dispersive energy contribution; and \tilde{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: $\varepsilon^{A,BI}$ (the association energy) and $k^{A,Bi}$ (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:

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

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

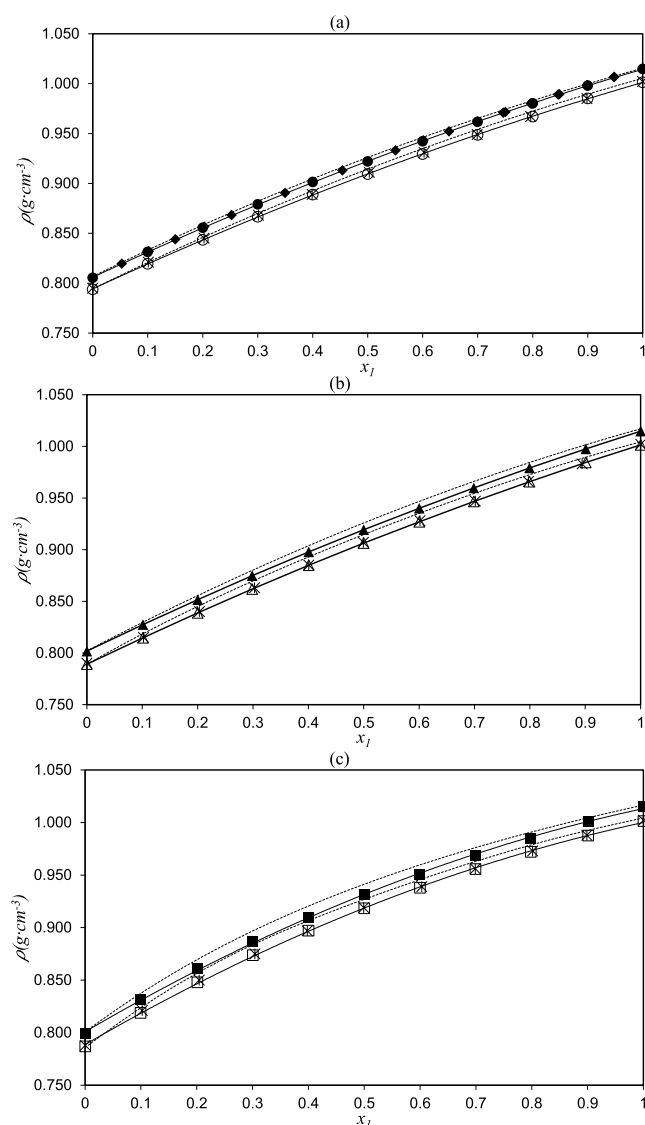


Figure 3. Experimental values of density, ρ , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), at 298.15 K: (●), this work; (◆), Mozo et al.⁷⁷ at 313.15 K; (○), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;⁷⁸ (b) 2-(2-methoxyethoxy)ethanol (1) + 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:

[0.009–0.15%], [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 , v , 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

Table 8. Sets of Parameters A_i , with Standard Deviations σ , Needed for Adjustment of Dynamic and Kinematic Viscosities, (η , ν), 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} |
| ν | 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} |
| ν | 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} |
| ν | 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) + propan-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

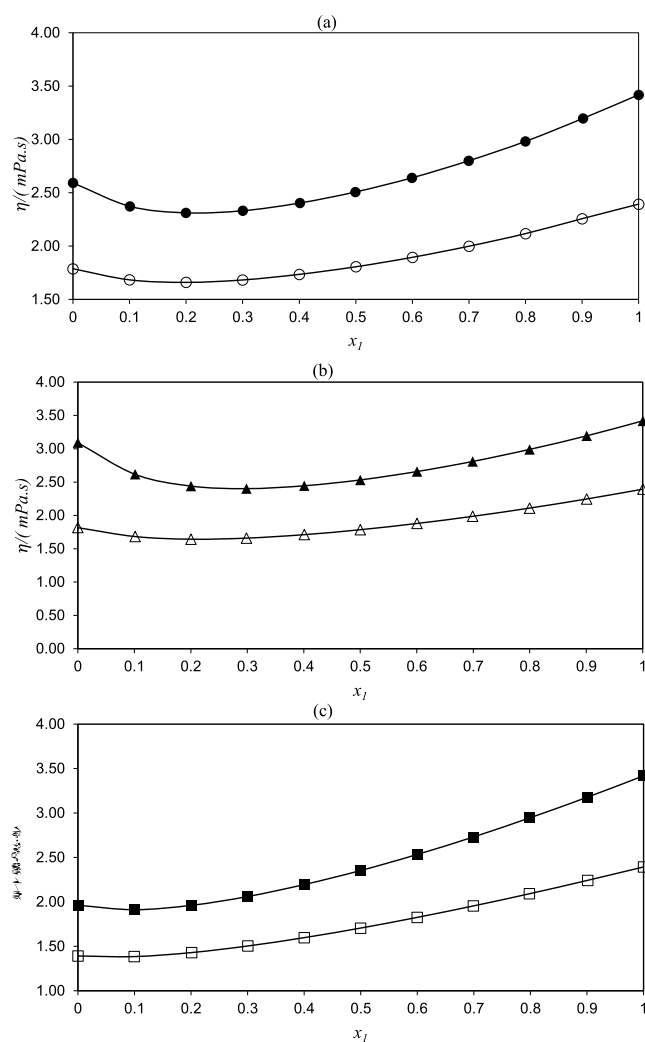


Figure 4. Experimental values of dynamic viscosity, η , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (●), this work at 298.15 K; (○), this work at 313.15 K; (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 298.15 K; (△), this work at 313.15 K; and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

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 , ν), Density, ρ , and Refractive Index, n_D . Experimental results of η , ν , 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 , ν , 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 ν values

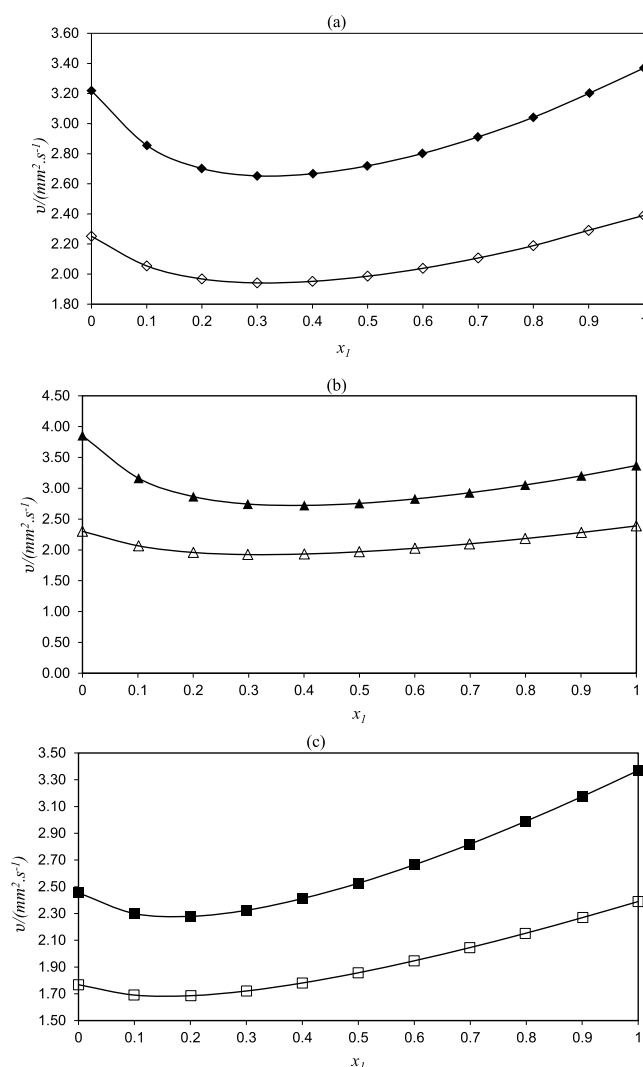


Figure 5. Experimental values of kinematic viscosity, ν , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (◆), this work at 298.15 K; (◇), this work at 313.15 K; (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); (▲), this work at 298.15 K; (△), this work at 313.15 K; 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.

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

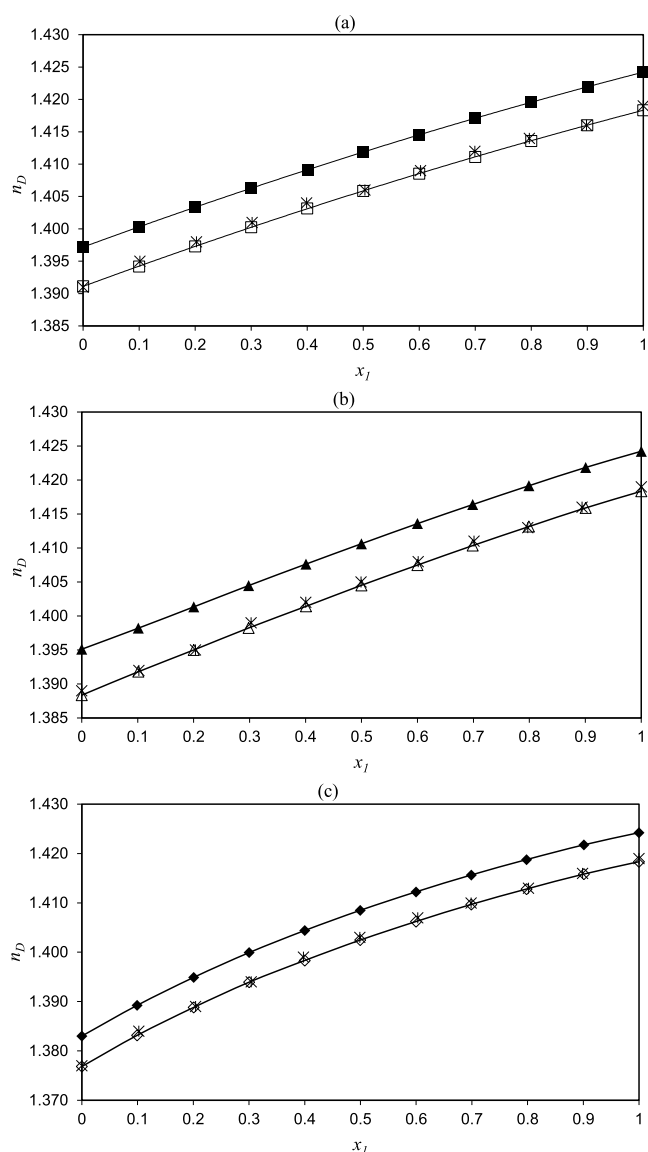


Figure 6. Experimental values of refractive index, n_D , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2), at 298.15 K; (■), this work, at 313.15 K; (□), this work (Cyrillic capital letter zhe with descender), Belhadj et al.;⁷⁸ (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (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.

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), +

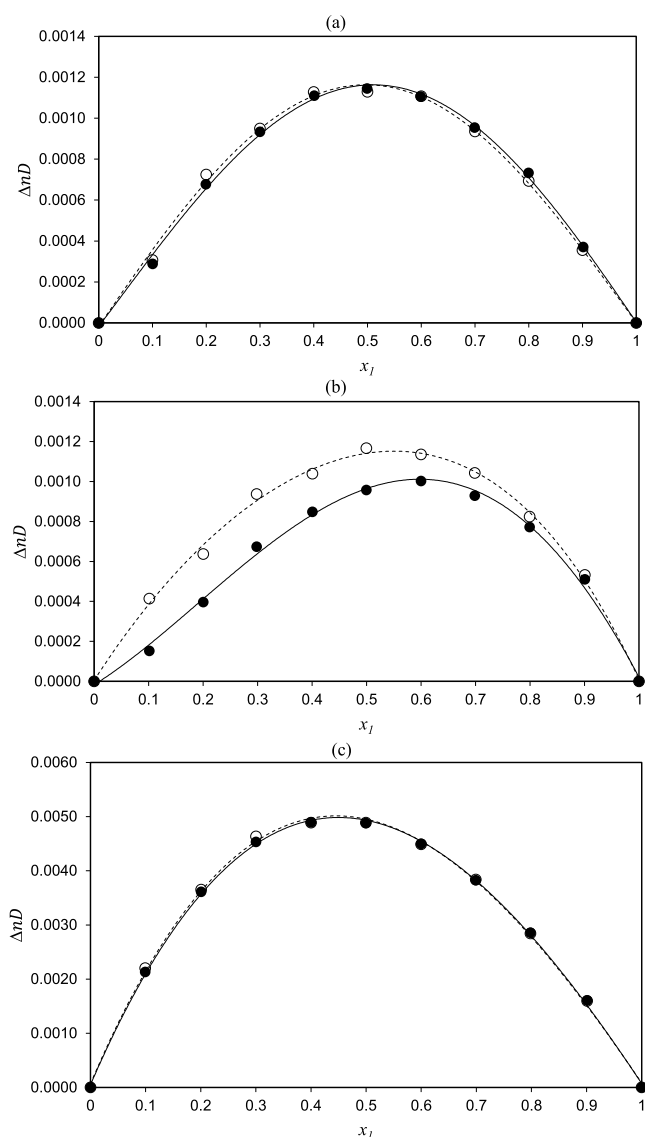


Figure 7. Calculated values of deviations in refractive index, Δn_D , as a function of x_1 for: (a) 2-(2-methoxyethoxy)ethanol (1) + butan-1-ol (2); (b) 2-(2-methoxyethoxy)ethanol (1) + butan-2-ol (2); and (c) 2-(2-methoxyethoxy)ethanol (1) + propan-1-ol (2). At temperatures: (●), 298.15 K and (○), 313.15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

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 [Å] | ϵ/k [K] | e^{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 |

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:

$$\Delta n_D = n_D - \sum_{i=1}^N x_i n_{Di} \quad (18)$$

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 , v , 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.

AUTHOR INFORMATION

Corresponding Author

Mohamed Lifi – Grupo de Energía, Economía y Dinámica de Sistemas (GEEDS), Universidad de Valladolid, Valladolid 47011, Spain; orcid.org/0000-0002-5426-6977; Email: mohamed.lifi@uva.es

Authors

Illham Abala – Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida 24000, Morocco; orcid.org/0000-0003-2543-9709

Raúl Briones-Llorente – Energy Engineering Research Group (iENERGÍA), Department of Mathematics and Computing, Faculty of Science, University of Burgos, Burgos 09001, Spain
Natalia Muñoz-Rujas – Departamento de Ingeniería Electromecánica, Escuela Politécnica Superior, Universidad de Burgos, Burgos 09006, Spain; orcid.org/0000-0003-2185-1392

Fernando Aguilar – Departamento de Ingeniería Electromecánica, Escuela Politécnica Superior, Universidad de Burgos, Burgos 09006, Spain; orcid.org/0000-0002-2982-9053

Fatima Ezzahrae M'hamdi Alaoui – Energy Laboratory, Faculty of Sciences, Abdelmalek Essaadi University, Tetouan 93002, Morocco

Complete contact information is available at: <https://pubs.acs.org/10.1021/acs.jced.3c00320>

Notes

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LIST OF SYMBOLS

H^E : excess enthalpy; η : dynamic viscosity; v : 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; $\max|\Delta H^E|$: absolute difference maximum; $\max(|\Delta H^E|/H^E)$: maximum relative deviation; rms: root-mean-square deviation

REFERENCES

- (1) Tchung-Ming, S.; Vinot, S. Les énergies pour le transport: avantages et inconvénients *Innovation Energy Environment*, 2009.
- (2) Bhupendra, S. C.; Ram, K. S.; Cho, H. M.; Lim, H. C. Practice of diesel fuel blends using alternative fuels: A review. *Renewable Sustainable Energy Rev.* **2016**, *59*, 1358–1368.
- (3) Zhang, Y.; Boehman, A. L. Oxidation of 1-butanol and a mixture of n-heptane/1-butanol in a motored engine. *Combust. Flame* **2010**, *157*, 1816–1824.
- (4) Lifi, M.; Muñoz-Rujas, N.; Montero, E. A.; Negadi, L.; Aguilar, F.; M'hamdi Alaoui, F. E. Excess molar enthalpy measurement and modelling of (oxygenated compounds + hydrocarbon) mixtures: Binary and ternary mixtures containing 2-(2-methoxyethoxy)ethanol, 1-hexene and cyclohexane at (298.15 and 313.15) K. *J. Chem. Thermodyn.* **2020**, *149*, No. 106171.
- (5) Lifi, M.; Muñoz-Rujas, N.; Montero, E. A.; Chhiti, Y.; Aguilar, F.; M'hamdi Alaoui, F. E. Measurement and Modeling of Excess Molar Enthalpies of Binary Mixtures Involving Hydrocarbon Components of Fuel. *J. Chem. Eng. Data* **2020**, *65* (2), 717–724.
- (6) Lifi, M.; Lorenzo, J.; Aguilar, F.; Muñoz-Rujas, N.; Montero, E. A.; Chhiti, Y.; M'hamdi Alaoui, F. E. Excess enthalpy, density, speed of sound and refractive index of binary mixtures {2-(2-ethoxyethoxy)-ethanol + 1-hexene, or cyclohexane, or methylcyclohexane at (298.15 and 313.15) K: Application of the PPR-78 cubic equation of state, NRTL and UNIQUAC models. *J. Chem. Thermodyn.* **2021**, *153*, No. 106306.
- (7) Aitbelale, R.; Abala, I.; Lifi, M.; Chhiti, Y.; M'hamdi Alaoui, F. E.; Sahib Eddine, A. High-Pressure Thermodynamic Properties of Fatty Acids Methyl Esters as Renewable Fuel. *Chem. Res. J.* **2020**, *5*, 242–260.
- (8) Lifi, M.; Lorenzo-Núñez, J.; Aguilar, F.; Muñoz-Rujas, N.; Montero, E. A.; Chhiti, Y.; M'hamdi Alaoui, F. E. Experimental Data of Thermophysical Properties of Mixtures of Oxygenated Additives + Hydrocarbon in Fuels and Biofuels: Application of Perturbed Chain-

- Statistical Associating Fluid and Peng–Robinson Equations of State. *J. Chem. Eng. Data* **2021**, *66* (3), 1475–1500.
- (9) Abala, I.; Lifi, M.; M'hamdi Alaoui, F. E.; Muñoz-Rujas, N.; Aguilar, F.; Montero, E. A. Density, Speed of Sound, Isentropic Compressibility, and Refractive Index of Ternary Mixtures of Oxygenated Additives and Hydrocarbons (Dibutyl Ether + 1-Butanol + Toluene or Cyclohexane) in Fuels and Biofuels: Experimental Data and PC-SAFT Equation-of-State Modeling. *J. Chem. Eng. Data* **2021**, *66* (3), 1406–1424.
- (10) Lifi, M.; Bazile, J.-P.; Muñoz-Rujas, N.; Galliero, G.; Aguilar, F.; Daridon, J.-L. Density, Viscosity and Derivative Properties of Diethylene Glycol Monoethyl Ether Under High Pressure and Temperature. *J. Chem. Eng. Data* **2021**, *66* (3), 1457–1465.
- (11) Abala, I.; Lifi, M.; M'hamdi Alaoui, F. E.; Muñoz-Rujas, N.; Aguilar, F.; Montero, E. A. Experimental data and Modeling of Liquid Density, Speed of Sound, Refractive Index and Derivative Properties of Ternary Mixtures Dibutyl Ether + 1-Butanol + Heptane or + Methylcyclohexane: Application of PC-SAFT Equation of State. *J. Chem. Thermodyn.* **2021**, *161*, No. 106549.
- (12) Lifi, M.; Montero, E. A.; Deshayes, L.; Muñoz-Rujas, N.; Chhiti, Y.; M'hamdi Alaoui, F. E.; Aguilar, F. In *Measurement and Modeling of Excess Enthalpies of Hydrocarbon Mixtures: Alkene + Alkane or + Cycloalkane at 313.15 K*, 5th International Conference on Renewable Energies for Developing Countries, REDEC, 2020; 9163877.
- (13) Abala, I.; Lifi, M.; Chhiti, Y.; Aitbelale, R.; M'hamdi Alaoui, F. E.; El khouakhi, M.; Deshayes, L. In *Estimation of PC-SAFT Equation of State Parameters of Hydrocarbons, Alcohols and Ethers*, 5th International Conference on Renewable Energies for Developing Countries, REDEC, 2020; 9163834.
- (14) Lifi, M.; Rubio-Pérez, G.; Lifi, H.; Muñoz-Rujas, N.; Aguilar, F.; M'hamdi Alaoui, F. E. Excess properties of mixtures containing 2-(2-ethoxyethoxy)ethanol, methylcyclohexane, cyclohexane and 1-hexene as fuel representative. *J. Chem. Thermodyn.* **2023**, *177*, No. 106933.
- (15) Gross, J.; Sadowski, G. Application of the perturbed-chain SAFT equation of state to associating systems. *Ind. Eng. Chem. Res.* **2002**, *41*, 5510–5515.
- (16) Gross, J.; Sadowski, G. Perturbed chain SAFT: An equation of state based on a perturbation theory for chain molecules. *Ind. Eng. Chem. Res.* **2001**, *40*, 1244–1260.
- (17) Redlich, O.; Kister, A. T. Algebraic Representation of Thermodynamic Properties and Classification of Solutions. *Ind. Eng. Chem.* **1948**, *40*, 345–348.
- (18) Abbott, M. M.; Van Ness, H. C. Vapor – liquid equilibrium: Part III. Data reduction with precise expressions for G^E . *AIChE J.* **1975**, *21*, 62–71.
- (19) Abrams, D. S.; Prausnitz, J. M. Statistical Thermodynamics of Liquid Mixtures: A New Expression for the Excess Gibbs Energy of Partly or Completely Miscible Systems. *AIChE J.* **1975**, *21*, 116–128.
- (20) Mozo, I.; García de la Fuente, I.; Gonzalez, J. A.; Cobos, J. C. Thermodynamics of Mixtures Containing Alkoxyethanols. XXIV. Densities, Excess Molar Volumes, and Speeds of Sound at (293.15, 298.15, and 303.15) K and Isothermal Compressibilities at 298.15 K for 2-(2-Alkoxyethoxy)ethanol + 1-Butanol Systems. *J. Chem. Eng. Data* **2007**, *52*, 2086–2090.
- (21) Kinart, C. M.; Nowak, K.; Kinart, W. J. Volumetric properties of binary mixtures of alkoxyethanols with ethyl tert-butyl ether at various temperatures. *J. Chem. Thermodyn.* **2005**, *37*, 423–429.
- (22) Kim, J.; Kim, M. Excess Molar Enthalpies and Excess Molar Volumes for the Binary Mixtures {1, 2-dichloropropane + 2-(2-methoxyethoxy) ethanol, and + 2-(2-ethoxyethoxy) ethanol} at 298.15 K. *Korean Chem. Eng. Res.* **2006**, *44*, 444–452.
- (23) Riddick, J. A.; Bunger, W. B.; Sakano, T. K. *Organic Solvents: Physical Properties and Methods of Purification*, 4th ed.; Wiley: United States, 1986.
- (24) Pal, A.; Kumar, H.; Kumar, A.; Dass, G. Excess molar volumes and viscosities of mixtures of some n-alkoxyethanols with dialkyl carbonates at 298.15 K. *Fluid Phase Equilib.* **1999**, *166*, 245–258.
- (25) Carmona, F. J.; Antonio Gonzalez, J.; García de la Fuente, I.; Carlos Cobos, J. Thermodynamic properties of n-alkoxyethanols + organic solvent mixtures. *Thermochim. Acta* **2004**, *409*, 169–175.
- (26) Carmona, F. J.; Gonzalez, J. A.; García de la Fuente, I.; Cobos, J. C. Thermodynamic Properties of N-Alkoxyethanols + Organic Solvent Mixtures. X. Liquid–Liquid Equilibria of Systems Containing 2-Methoxyethanol, 2-(2-Methoxyethoxy)ethanol or 2-(2-Ethoxyethoxy)ethanol, and Selected Alkanes. *J. Chem. Eng. Data* **1999**, *44*, 892–895.
- (27) Francesconi, R.; Castellari, C.; Comelli, F. Excess Molar Enthalpies and Excess Molar Volumes of Diethyl Carbonate + Somen-Alkoxyethanols at (298.15 and 313.15) K. *J. Chem. Eng. Data* **1999**, *44*, 1373–1378.
- (28) Pal, A.; Sharma, S. Viscosities and Densities of Some-nAlkoxyethanols with Trichloroethylene and Tetrachloroethylene at 298.15 K. *J. Chem. Eng. Data* **1998**, *43*, 21–24.
- (29) Dhondge, S. S.; Pandhurnekar, C. P.; Sheikh, S.; Deshmukh, D. W. Volumetric and viscometric study of aqueous binary mixtures of some glycol ethers at T = (275.15 and 283.15) K. *J. Chem. Thermodyn.* **2011**, *43*, 1961–1968.
- (30) Pal, A.; Sharma, S. Excess Molar Volumes and Viscosities of Binary Liq. Mixt. Of Ethylene Glycol Diethyl Ether + Ethylene Glycol Monomethyl, + Diethylene Glycol Monomethyl, + Triethylene Glycol Monomethyl Ethers at 298.15 and 308.15 K. *J. Chem. Eng. Data* **1999**, *44*, 1067–70.
- (31) Kinart, C. M.; Cwiklinska, A.; Kinart, W. J.; Bald, A. Viscosities of some n-alkoxyethanols with ethyl tert-butyl ether at T = (293.15, 298.15 and 303.15) K. *J. Mol. Liq.* **2006**, *126*, 135–139.
- (32) Riddick, J. A.; Bunger, W. S.; Sakano, T. *Techniques of Chemistry*, 4th ed.; John Wiley and Sons: NewYork, 1986; Vol. II.
- (33) Belhadj, D.; Bahadur, I.; Negadi, A.; Muñoz-Rujas, N.; Montero, E.; Negadi, L. Thermodynamic, Ultrasonic, and Transport Study of Binary Mixtures Containing 2-(2-Methoxyethoxy)ethanol and Alcohols at (293.15–323.15) K. *J. Chem. Eng. Data* **2020**, *65* (11), 5192–5209.
- (34) Comelli, F.; Francesconi, R.; Castellari, C. Excess molar enthalpies of binary mixtures containing propylene carbonate + some n-alkoxy- and n-alkoxyethoxy-ethanols at 288.15, 298.15, and 313.15 K. *Thermochim. Acta* **2000**, *354*, 89–97.
- (35) Tseng, Y.-M.; Thompson, R. Densities and Refractive Indices of Diethylene Glycol Ether-Water Solutions. *J. Chem. Eng. Data* **1962**, *7*, 483.
- (36) Kurtz, S. S.; Camin, D. L.; Thompson, A. R. Refractive index + density slope associated with volume change on mixing. *J. Chem. Eng. Data* **1965**, *10*, 335–339.
- (37) Carmona, F. J.; Gonzalez, J. A.; Garcia de la Fuente, I.; Cobos, J. C. Thermodynamic Prop. of N-Alkoxyethanols + Org. Solvent Mixtures. X. Liq.-Liq. Equil. of Syst. Containing 2-Methoxyethanol, 2-(2-Methoxyethoxy)ethanol or 2-(2-Ethoxyethoxy)ethanol and Selected Hydrocarbons. *J. Chem. Eng. Data* **1999**, *44*, 892–5.
- (38) Dhondge, S. S.; Pandhurnekar, C. P.; Parwate, D. V. Thermodynamic and optical studies of some ethylene glycol ethers in aqueous solutions at T= 298.15 K. *J. Chem. Thermodyn.* **2009**, *41*, 577–585.
- (39) Singh, T.; Kumar, A. Volumetric behaviour of 1-Butyl-3-Methyl imidazolium hexafluorophosphate with ethylene glycol derivatives: Application of Prigogine-Flory-Patterson theory. *J. Mol. Liq.* **2010**, *153*, 117–123.
- (40) Yang, C.; Lai, H.; Liu, Z.; Ma, P. Density and Viscosity of Binary Mixtures of Diethyl Carbonate with Alcohols at (293.15 to 363.15) K and Predictive Results by UNIFAC-VISCO Group Contribution Method. *J. Chem. Eng. Data* **2006**, *51*, 1345–1351.
- (41) Rodríguez, A.; Canosa, J.; Tojo, J. Density, refractive index, and speed of sound of binary mixtures (diethyl carbonate + alcohols) at several temperatures. *J. Chem. Eng. Data* **2001**, *46*, 1506–1515.
- (42) Aminabhavi, T. M.; Gopalakrishna, B. Densities, viscosities, and refractive indices of bis(2-methoxyethyl) ether + cyclohexane or + 1,2,3,4-tetrahydronaphthalene and of 2-ethoxyethanol + propan-1-ol,

+ propan-2-ol, or + butan-1-ol. *J. Chem. Eng. Data* **1995**, *40*, 462–467.

(43) Vallés, C.; Perez, E.; Cardoso, M.; Dominguez, M.; Mainar, A. M. Excess enthalpy, density, viscosity, and speed of sound for the mixture tetrahydropyran + 1-butanol at (283.15, 298.15, and 313.15) K. *J. Chem. Eng. Data* **2004**, *49*, 1460–1464.

(44) Rodríguez, A.; Canosa, J.; Dominguez, A.; Tojo, J. Dynamic viscosities of diethyl carbonate with linear and secondary alcohols at several temperatures. *J. Chem. Eng. Data* **2004**, *49*, 157–162.

(45) Indraswati, N. M.; Mudjijati; Wicaksana, F.; Hindarso, H.; Ismadji, S. Measurements of density and viscosity of binary mixtures of several flavor compounds with 1-butanol and 1-pentanol at 293.15 K, 303.15 K, 313.15 K, and 323.15 K. *J. Chem. Eng. Data* **2001**, *46*, 696–702.

(46) Djojoputro, H.; Ismadji, S. Density and viscosity of binary mixtures of ethyl-2 methylbutyrate and ethyl hexanoate with methanol, ethanol, and 1-propanol at (293.15, 303.15, and 313.15) K. *J. Chem. Eng. Data* **2005**, *50*, 1343–1347.

(47) Mokhtarani, B.; Shariif, A.; Mortaheb, H. R.; Mirzaei, M.; Mafi, M.; Sadeghian, F. Density and viscosity of 1-butyl-3-methylimidazolium nitrate with ethanol, 1-propanol, or 1-butanol at several temperatures. *J. Chem. Thermodyn.* **2009**, *41*, 1432–1438.

(48) Spasojević, V. D.; Djordjević, B. D.; Serbanovic, S. P.; Radovic, I. R.; Kijeveanin, M. L. Densities, Refractive Indices, Viscosities, and Spectroscopic Study of 1-Amino-2-propanol + 1-Butanol and + 2-Butanol Solutions at (288.15 to 333.15) K. *J. Chem. Eng. Data* **2014**, *59*, 1817–1829.

(49) Loras, S.; Monton, B. J.; España, F. Vapor-Liquid Equilibria for the Binary Systems of Methylcyclohexane with 1-Propanol, 2-Propanol, 1-Butanol, and 2-Butanol at 101.3 kPa. *J. Chem. Eng. Data* **1997**, *42*, 914–918.

(50) TRC Tables, *Thermodynamic Tables*, version 2.0 Thermodynamics Research Center: Houston, TX, 1995.

(51) Almasi, M.; Iloukhani, H. Densities, Viscosities, and Refractive Indices of Binary Mixtures of Acetophenone and 2-Alkanols. *J. Chem. Eng. Data* **2010**, *55*, 1416–1420.

(52) Martínez, S.; Garriga, R.; Perez, P.; Gracia, M. Densities and viscosities of binary mixture of butanone with butanol isomers at several temperatures. *Fluid Phase Equilib.* **2000**, *168*, 267–279.

(53) Lomte, S. B.; Bawa, M. J.; Lande, M. K.; Arbad, B. R. Densities and Viscosities of Binary Liquid Mixtures of 2-Butanone with Branched Alcohols at (293.15 to 313.15) K. *J. Chem. Eng. Data* **2009**, *54*, 127–130.

(54) Ortega, J. Densities and Refractive Indices of Pure Alcohols as a Function of Temperature. *J. Chem. Eng. Data* **1982**, *27*, 312–7.

(55) O'Brien, R. N.; Quon, D. Refractive Index of Some Alcohols and Saturated Hydrocarbons at 6328 Å. *J. Chem. Eng. Data* **1968**, *13*, 517.

(56) Kijeveanin, M. L.; Radovic, I. R.; Djordjevic, B. D.; Tasic, A. Z.; Serbanovic, S. P. Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K. *Thermochim. Acta* **2011**, *525*, 114–28.

(57) *Selected Values of Properties of Chemical Compounds, Data Project, Thermo-dynamics Research Center*; Texas A&M University: College Station, TX, 1980.

(58) Ayranci, E.; Akgul, G. Apparent Molar Volumes and Viscosities of Lauric, Palmitic, and Stearic Acids in 2-Butanol at (20, 30, 40, and 60) °C. *J. Chem. Eng. Data* **2003**, *48*, 56–60.

(59) Bravo-Sánchez, M. G.; Iglesias-Silva, G. A.; Estrada-Baltazar, A.; Hall, K. R. Densities and Viscosities of Binary Mixtures of n-Butanol with 2-Butanol, Isobutanol, and tert-Butanol from (303.15 to 343.15) K. *J. Chem. Eng. Data* **2010**, *55*, 2310–2315.

(60) Mesquita, F. M. R.; Feitosa, F. X.; Aznar, M.; SantAna, H. B. D.; Santiago-Aguiar, R. S. Density, Viscosities, and Excess Properties for Binary Mixtures of Sulfolane + Alcohols and Sulfolane + Glycols at Different Temperatures. *J. Chem. Eng. Data* **2014**, *59*, 2196–2206.

(61) Živković, N. V.; Serbanovic, S. S.; Kijeveanin, M. L.; Živkovic, E. M. Volumetric and Viscometric Behavior of Binary Systems 2-

Butanol + PEG 200, + PEG 400, + Tetraethylene Glycol Dimethyl Ether, and + N-Methyl-2-pyrrolidone. *J. Chem. Eng. Data* **2013**, *58*, 3332–3341.

(62) Martínez, S.; Garriga, R.; Perez, P.; Gracia, M. Densities and viscosities of binary mixtures of butanenitrile with butanol isomers at several temperatures. *J. Chem. Eng. Data* **2000**, *45*, 1182–1188.

(63) Chandra Sekhar, M.; Mohan, T. M.; Krishna, T. V.; Venkatesulu, A.; Kumar, K. S. Density, Refractive Index, Speed of Sound and Computational Studies of Intermolecular Interactions in Binary Mixtures of 2-Chloroaniline with Butanols (1-Butanol, 2-Butanol) at T = (303.15–318.15) K. *J. Solution Chem.* **2015**, *44*, 237–263.

(64) Pang, F.-M.; Seng, C.-E.; Teng, T.-T.; Ibrahim, M. H. Densities and viscosities of aqueous solutions of 1-propanol and 2-propanol at temperatures from 293.15 to 333.15 K. *J. Mol. Liq.* **2007**, *136*, 71–78.

(65) Mikhail, S. Z.; Kimel, W. R. Densities and Viscosities of 1-Propanol-Water Mixtures. *J. Chem. Eng. Data* **1963**, *8*, 323–328.

(66) Belhadji, D.; Bahadur, I.; Negadi, A.; Muñoz-Rujas, N.; Montero, E.; Negadi, L. Thermodynamic, Ultrasonic, and Transport Study of Binary Mixtures Containing 2-(2-Methoxyethoxy)ethanol and Alcohols at (293.15–323.15) K. *J. Chem. Eng. Data* **2020**, *65*, 5192.

(67) Aguilar, F.; Alaoui, F. E. M.; Alonso-Tristán, C.; Segovia, J. J.; Villamañán, M. A.; Montero, E. A. Excess enthalpies of binary and ternary mixtures containing dibutyl ether (DBE), cyclohexane and 1-butanol at 298.15 K. *J. Chem. Eng. Data* **2009**, *54* (6), 1672–1679.

(68) Expression of the Uncertainty of Measurement in Calibration, European cooperation for Accreditation, EA4–02, 1999.

(69) Bevington, P. R.; Robinson, D. K. *Data Reduction and Error Analysis for the Physical Sciences*; WCD/McGraw-Hill, Boston, Mass, 1992.

(70) Abala, I.; M'hamdi Alaoui, F. E.; Sahib Eddine, A.; Aguilar, F.; Muñoz Rujas, N.; Montero, E. (ρ , VE, T) Measurements of the Ternary Mixture (Dibutyl Ether + 1-Heptanol + Heptane) at Temperatures up to 393.15 K and Pressures up to 140 MPa and Modeling Using the Peng–Robinson and PC-SAFT Equations of State. *J. Chem. Eng. Data* **2019**, *64* (9), 3861–3873.

(71) Abala, I.; M'hamdi Alaoui, F. E.; Chhiti, Y.; Sahib Eddine, A.; Muñoz Rujas, N.; Aguilar, F. Density of biofuel mixtures (Dibutyl ether + Heptane) at temperatures from (298.15e393.15) K and at pressures up to 140 MPa: Experimental data and PC-SAFT modelling. *Fluid Phase Equilib.* **2019**, *491*, 35–44.

(72) Grenner, A.; Kontogeorgis, G. M.; von Solms, N.; Michelsen, M. L. Modeling phase equilibria of alkanols with the simplified PC-SAFT equation of state and generalized pure compound parameters. *Fluid Phase Equilib.* **2007**, *258* (1), 83–94.

(73) Ahmadi, S.; Almasi, M. Experimental and modeling study of diisopropyl ether and 2-alkanol; PC-SAFT model and free volume theory. *J. Chem. Thermodyn.* **2020**, *142*, No. 106025.

(74) Cobos, J. C.; Casanova, C. Excess Enthalpies of Some Cellosolves With 1-Butanol at 298.15 K. *Fluid Phase Equilib.* **1985**, *20*, 155–60.

(75) Qian, J. W.; Privat, R.; Jaubert, J.-N.; Duchet-Suchaux, P. Enthalpy and Heat Capacity Changes on Mixing: Fundamental Aspects and Prediction by Means of the PPR78 Cubic Equation of State. *Energy Fuels* **2013**, *27* (11), 7150–7178.

(76) Reddy, K. V. R.; Rambabu, K.; Krishnaiah, A.; Ramakrishna, M. Excess enthalpies of binary mixtures containing Methyl Cellosolve and aliphatic alcohols. *Fluid Phase Equilib.* **1995**, *103*, 251–256.

(77) Mozo, I.; de la Fuente, I. G.; Gonzalez, J. A.; Cobos, J. C. Thermodynamics of Mixtures Containing Alkoxyethanols. XXIV. Densities, Excess Molar Volumes, and Speeds of Sound at (293.15, 298.15, and 303.15) K and Isothermal Compressibilities at 298.15 K for 2-(2-Alkoxyethoxy)ethanol + 1-Butanol Systems. *J. Chem. Eng. Data* **2007**, *52*, 2086–2090.

(78) Belhadji, D.; Bahadur, I.; Negadi, A.; Munoz-Rujas, N.; Montero, E.; Negadi, L. Thermodynamic, Ultrasonic, and Transport Study of Binary Mixtures Containing 2-(2-Methoxyethoxy)ethanol

and Alcohols at (293.15–323.15) K. *J. Chem. Eng. Data* **2020**, *65*, 5192–5209.