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A systematic study on volumetric and transport properties of binary systems 1-propanol + n-hexadecane, 1-butanol + n-hexadecane and 1-propanol + ethyl oleate at different temperatures: experimental and modeling

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Abstract

Densities (ρ), viscosities (η), speed of sounds (u) and refractive indices (n_D) at temperature range (293.15-343.15) K with 5 K interval, for three binary mixtures (1-propanol + *n*-hexadecane, 1-butanol + *n*-hexadecane and 1-propanol + ethyl oleate), were measured at atmospheric pressure. Based on the corresponding experimental data, excess molar volume (V^E), viscosity deviation ($\Delta\eta$) and deviation in refractive index (Δn_D) have been calculated. Beside these properties, molar excess Gibbs free energies of activation of viscous flow ($\Delta^* G^E$) and deviation in isentropic compressibility ($\Delta\kappa_s$) were calculated from measured density, viscosity and speed of sound data. The excess / deviation functions have been fitted by Redlich-Kister equation and discussed in terms of molecular interactions existing in the mixtures. Viscosity modeling was performed using four models: UNIFAC-VISCO, ASOG-VISCO, Teja-Rice and McAllister. Experimental viscosity data have been used to determine new binary UNIFAC-VISCO and ASOG-VISCO interaction parameters and the interaction parameters for correlation models by applying some optimization technique. For all systems, positive deviations were observed for the excess molar volumes in the whole concentration range. A negative deviation and an inversion sign for the excess dynamic viscosity were observed in the systems of 1-butanol + *n*-hexadecane and 1-propanol + *n*-hexadecane, respectively, while positive deviation was observed for 1-propanol + ethyl oleate mixture. The results of viscosity modeling showed that four-body McAllister models are suitable to describe viscosities for all systems and temperatures with maximum percentage deviations (PD_{max}) less than 0.5 %.

Key words: Density; Viscosity; Refractive index; Speed of sound; Viscosity modeling; Group contribution parameters.

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