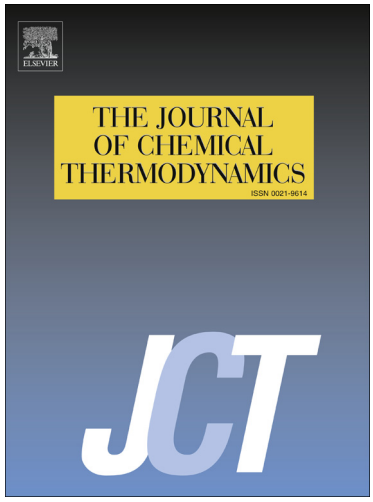

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Excess properties and isobaric vapor-liquid equilibrium at sub-atmospheric pressures of binary (1,2-propanediol +1,3-propanediol) system : Measurement and Modelling

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Abstract

Experimental vapor-liquid equilibrium data were obtained at sub-atmospheric pressures of 6.66, 13.33, 19.99, 26.66, 33.33, 39.99 and 46.66 kPa for the binary system 1,2-propanediol + 1,3-propanediol over the entire composition range using Swietoslasky-type ebulliometer. Wilson and NRTL activity coefficient models were used to correlate the experimental VLE data for which optimum binary interaction energy parameters are reported. NRTL model fitted well with experimental data as compared to Wilson model. Density and refractive indices of binary mixtures are also reported along with their excess properties such as excess molar volumes (V_m^E), excess refractive index (n^E), partial molar volume ($\bar{V}_i$), apparent molar volume ($V_{\phi i}$), and excess partial molar volume ($\bar{V}_i^E$) at different temperatures (293.15 to 318.15) K. The excess molar volumes data were used to test the applicability of Prigogine-Flory-Patterson theory and refractive index values to test different mixing rules.

Keywords: 1,2-Propanediol, 1,3-Propanediol, Vapor-Liquid Equilibrium, Excess properties, PFP theory, Mixing rules.

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1. Introduction

1,2-Propanediol and 1,3-Propanediol are members of alkanediol family, which are inexhaustible significant products produced by a novel pathway such as hydrogenolysis of glycerol [1]. 1,2-Propanediol (1,2-pd) is a valuable intermediate for manufacturing polyester resins, which is used as industrial solvent, as an additive in food, cosmetic and pharmaceutical industries. 1,3-Propanediol (1,3-pd) has an ability to replace ethylene glycol and butylene glycol in the process for synthesis of polyesters and polyurethanes [2]. It is an important raw material for polytrimethylene terephthalate (3GT) polyester, which is widely used in textile industries. Knowledge of vapor-liquid equilibrium (VLE) data of 1,2-pd + 1,3-pd is necessary for separation of components from their mixtures. The study of thermophysical properties such as density and refractive index of mixtures helps in understanding not only the interactions between solute-solute, solvent-solvent and solute-solvent, but also accounts for packing effects which arise due to differences in sizes of molecules [3]. There is an enormous significance to investigate the VLE behavior and thermodynamic properties of alkanediol mixtures as it plays an important role in industries. Different researchers have investigated the volumetric, viscometric and acoustic properties of pure alkanediols as well as mixtures. Mokbel et al. [4] have reported the vapor pressure data of 1,3-propanediol and 1,2,3-propanetriol at pressures (6 to 45) kPa and for two mixtures, glycerol + water and glycerol