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Thermodynamic insights on the viscometric and volumetric properties of binary mixtures of ketals and polyols

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Abstract

Recently, solketal (Sk) and glycerol formal (GF) have appeared as alternatives for the chemical valorization of glycerol (Gly), a by-product derived from the biodiesel industry. Sk and GF are versatile products with increasing interest in several industries due to their attractive properties, particularly in foods, pharmaceuticals and products of the fast moving consumer goods industry. In addition, glycols like 1,2-propanediol (1,2-PD), ethylene glycol (EG) are also valuable chemicals whose production can also derive from the valorization of Gly.

Information on the viscometric and volumetric properties of these compounds is very scarce, yet simultaneously critical to assess potential industrial applications. Here the density and viscosity of the binary mixtures of {GF + 1,2-PD}, {GF + EG}, {GF + Gly}, {Sk + 1,2-PD}, {Sk + EG} and {Sk + Gly} are experimentally measured over the entire range of compositions at 298.15, 308.15 and 313.15 K and atmospheric pressure. Correlation of these properties to the Jouyban-Acree equation was made to explain their variation with composition and temperature. Furthermore, molar excess volumes and viscosity deviations are herein calculated and Redlich-Kister equations are employed to model the behaviour with composition. Finally, the experimental results are supported with quantum chemical calculations based on COSMO-RS method in order to shed light

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