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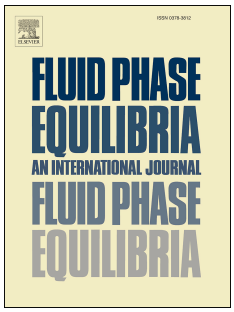

Guaiacol and its mixtures: New data and predictive models. Part 2: Gibbs energy of solvation

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Guaiacol and its mixtures: new data and predictive models. Part 2: Gibbs energy of solvation

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Abstract

Guaiacol is a model molecule for lignocellulosic biomass processing, and thus understanding its interactions with solvents is an important step when developing units for processing lignocellulosic biomass. In this work, activity coefficient measurements of different solvents (acetonitrile, ethanol, tetrahydrofuran) in guaiacol have been performed at different concentrations and temperatures. These measurements have been used to estimate the infinite dilution activity coefficients and the Gibbs energy of solvation of guaiacol in the different solvents, and of each solvent in guaiacol. These estimated values were compared to those obtained with different predictive models: UNIFAC DMD, Monte Carlo Molecular Simulation, COSMO-SAC and GC-PPC-SAFT. The predictions are in very good agreement with the Gibbs energies of solvation derived from experimental data. Some conclusions are also drawn regarding the inter and intramolecular hydrogen bonding in guaiacol and about its affinity with different solvents on the basis of the inter and intra molecular interactions taking place.

Keywords: activity coefficient; Gibbs energy of solvation; gas chromatography; GC-PPC-SAFT; Monte Carlo molecular simulation

1. Introduction

Lignocellulosic biomass (LCB) can be a potential resource for the production of different chemicalreagents and fuels. LCB usage will help to protect the environment and to reduce the dependence on fossil fuels, which is important for sustainable development of economics as well as for creation of new workplaces at the regional level and development of rural areas [1]. There is now a commitment from the chemical industry to develop new green chemistry-based processes [2-6], and LCB is called to play a major role as an alternative raw material. It has several advantages in comparison with fossil raw materials: renewable, widely available and better distributed throughout the world. As a matter of fact, lignocellulosescan be used to synthesizetargetmolecules for many applications, which are consistent with the principles of green chemistry [6]. However, the development of effective processes to