

Vapor-Liquid Equilibria and Water Activities of Aqueous Ionic Liquids with the Soft-SAFT EoS

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The unique physical properties of ionic liquids (ILs) make them valuable alternatives to traditional compounds for different applications. Aqueous ILs systems are of particular interest for different applications such as in absorption refrigeration and in separation and purification processes through the use of aqueous biphasic systems. The precise description of thermodynamic properties and phase equilibria of aqueous ionic liquid solutions is fundamental for a correct design and application of these processes. In this work, the soft-SAFT equation of state (EoS), a successful approach able to accurately describe the thermophysical properties and phase behavior of ILs and their mixtures, will be used to describe water activities and the vapor-liquid equilibrium (VLE) of a wide range of water + IL systems covering different families of ILs. The correct description of these properties provides new insights about aqueous ILs ideal behavior and solute-solvent interactions, and allows further model application to predict the behavior of other aqueous ILs. The information obtained will be used to discriminate among different sets of molecular soft-SAFT parameters for the ILs which have never been modeled using soft-SAFT.