Prediction of thermodynamics and fluid-phase behaviour of aqueous solutions of linear, branched, and cyclic amines

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Abstract

The SAFT-γ Mie group-contribution equation of state is used to represent the fluid-phase behaviour of aqueous solutions of a variety of linear, branched, and cyclic amines. New group interactions are developed in order to model the mixtures characterised by alkyl primary, secondary, and tertiary amine groups (NH2, NH, N), cyclic secondary and tertiary amine groups (cNH, cN), and cyclohexylamine groups (cCHNH, cCHN). The group-interaction parameters are estimated from appropriate experimental thermodynamic data for pure amines and selected mixtures. The fluid-phase behaviour of these mixtures can then be described over broad ranges of temperature, pressure, and composition. Liquid-liquid equilibria (LLE) bounded by lower critical solution temperatures (LCSTs) have been reported experimentally and are reproduced here with SAFT-γ Mie approach. The main feature of the approach is the ability to represent accurately the experimental data employed in the parameter estimation, a to predict the phase equilibria with the same set of parameters.

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