Prediction of Liquid-Liquid Multi-Component Equilibrium Systems Using COSMO-RS

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The Conductor-like screening model for real solvents (COSMO-RS) combines an electrostatic theory of locally interacting molecular surface descriptor with statistical thermodynamic methodology. The molecular surface descriptor, represented as sigma surfaces and profiles, were obtained from quantum chemical calculations using the program package Turbomole. Sigma profiles are used as input to the COSMO-RS method to calculate various thermodynamic properties of pure components and their mixtures.
In this study COSMO-RS method was employed to calculate liquid-liquid equilibrium involving multiple components. The results show the good prediction capabilities or the COSMO-RS method for various systems, in comparison with available experimental date.