

Phase Equilibria in Binary Mixtures of Propane and Phenanthrene: Experimental Data and Modeling with the GC-EOS

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Systems consisting of a volatile solvent composed of small molecules, such as propane, and a solute consisting of low volatile, complex molecules, such as poly-aromatic compounds, are known to show complex phase behavior. Multiphase fluid behavior may occur and also a solid phase can be present, which further increases the complexity of the phase diagrams. The present work focuses on binary mixtures consisting of propane + phenanthrene. This system shows type III phase behavior in the classification of Scott and Van Konynenburg. Various two-phase and three-phase equilibria were measured experimentally, including equilibria in the presence of solid phenanthrene. Based on the course of the various three-phase equilibria an estimation could be made for the location of the quadruple point solid phenanthrene-liquid-liquid-vapor. The Group Contribution Equation of State (GC-EoS) developed by Skjold-Jørgensen was applied to reproduce the experimental data points. Phenanthrene was considered as a single group for which pure group parameters had to be determined by fitting phenanthrene vapor pressure data. Interaction parameters between phenanthrene and the CH₃ and CH₂ groups in propane were fitted to propane-phenanthrene bubble point data. The GC-EoS was applied to calculate vapor and liquid phase fugacities which were required in the phase equilibria calculations. The fugacity of pure solid phenanthrene was related to the fugacity of the pure subcooled liquid using changes in Gibbs free energy and a thermodynamic cycle which proceeds from the subcooled liquid to the solid state and passes through the triple point. Good agreement between experimental and calculated phase equilibrium data was obtained with the GC-EoS.