# Derivative Properties of Pure Fluids and Binary Mixtures of N-Alkane and 1-Alkanols Through a Molecular-Based Equation of State

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Most of the molecular-based equations of state (EoSs) have been developed up-to-date for phase equilibria calculations. The molecular parameters of the equation are obtained by fitting to available phase equilibria experimental data and used, in a transferable manner, to predict the phase behavior of the system at different conditions. One of the most stringent tests that can be performed to this type of equations is its transferability to calculate thermodynamic properties with the molecular parameters obtained from phase equilibria calculations. Of special relevance are the heat capacities, inversion curves, speed of sound, etc., as the second derivatives are always more sensitive to errors than the original function.

The goal of this work was to check the capability of the molecular-based soft-SAFT equation [1] to calculate the main derivative properties of the n-alkane and the 1-alkanol families, in order to show the predictive power of this equation. Several compounds have been analyzed to show the influence of the chain length and the association effect. Different n-alkane-1-alkanol mixtures have been studied, calculating vapor-liquid equilibria and predicting heat capacities, compressibilities and speeds of sound in a broad range of thermodynamic conditions. The influence of the temperature and the pressure will also be discussed, as well as the finding of some pitfalls of the equation outside the range of applicability of the reference fluid term.

A renormalization-group treatment has also been included to improve results in the vicinity of the critical point. The procedure, based on White's work [2], was implemented in terms of recursion relations where the density fluctuations were successively incorporated [3]. The study of the behavior of derivative properties near the critical point becomes a final test to check the capabilities of soft-SAFT equation.

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