Temperature Dependence of the Heat Capacity and Vapor Pressure of Pure Self-Associated Liquids. a New Correlation Based on a Two State Association Model

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A recently reported (J. Chem. Phys., 2004, **120**, 6648) two state association model (TSAM) is reformulated to obtain an expression for the residual Gibbs free energy of pure self-associating liquids. From the proposed partition function, where association is considered a perturbation, a vapor pressure correlation was obtained, with a clear and separable non-specific contribution. The new formulation does not change the reported three or four parameter equation for calculating residual heat capacities, their values being determined solely from experimental heat capacity experimental data. Two new parameters are necessary to describe the non specific reference fluid Gibbs free energy. The resulting vapor pressure equation was fitted to experimental data for pure 1–alcohols, 1–thiols, 1–amines and carboxylic acids with very good agreement, up to the critical point.