Excess Gibbs Energy of Mixing (G^E) and Vapor-Liquid Equilibria (VLE) of Ethanol + Water: A Critical Evaluation and Recommended Values

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Literature experimental ethanol + water VLE data between 298 K and 500 K were fitted using activity-coefficient equations derived from Redlich-Kister and Legendre polynomial expansions of G^E. These data were tested for thermodynamic consistency vs. temperature using the Gibbs-Helmholtz equation for comparison to literature excess enthalpy of mixing (H^E) and excess heat capacity ($C_p{}^E$) data. Fugacity coefficients were computed from the second-virial equation. Priority was given to datasets that include pure-component vapor pressures measured in the same apparatus and with the same materials as the mixture experiments. The number of concentration-dependent terms needed to fit isothermal sets of VLE data was statistically tested to prevent overfitting of the data while retaining the needed statistically-significant number of fitting-equation terms. Thermodynamic consistency of isobaric *PTxy* (recirculating equilibrium still) data was examined using the Gibbs-Duhem equation and Barker-method fitting of the *PTx* part of the data as recommended by Kang, et al. A recommended temperature and composition dependent G^E equation and recommended tables of excess properties, VLE, and relative volatility are given. Recommended values for isobaric and isothermal azeotropic compositions are also presented.