

Liquid Renewable Fuels: Excess Thermodynamic Properties of Binary and Ternary Mixtures Containing ETBE, Cyclohexane and Toluene

J.J. Segovia^C, C.R. Chamorro, M.A. Villamañán^S, M.C. Martín and R.M. Villamañán
*Departamento de Ingeniería Energética y Fluidomecánica, Grupo de Termodinámica y Calibración
TERMOCAL, Universidad de Valladolid, Valladolid, Spain
josseg@eis.uva.es*

In the formulation of new renewable gasoline, bioethers and bioalcohols are used as blending agents for enhancing the octane number. These compounds also help fuels burn cleaner and more efficiently. Their effect is to make gasoline work harder, help engines last longer and reduce air pollution. To better understand and model it we started many years ago a research program on the thermodynamic characterization of ternary mixtures, as the simplest multicomponent system, containing oxygenated additives (ethers and alcohols) and different type of hydrocarbons (paraffins, cycloparaffins, aromatics, olefins).

The highest quality of thermodynamic data is required to improve the interaction parameters of the predictive models which are used in process simulation packages. The accuracy of a process simulation depends strongly on the thermodynamic models used to describe the physical behavior of the involved components.

An isothermal total pressure cell has been employed for measuring the vapor-liquid equilibrium of binary and ternary mixtures. The apparatus and static measuring technique are based on that by Van Ness and has been described in detail in the literature [1]. The equilibrium properties measured directly and their uncertainties are: injected volume ± 0.03 ml, temperature ± 10 mK and total pressure ± 5 Pa. A quasi-isothermal flow calorimeter designed in our laboratory by Segovia has been used to determine the excess enthalpies of the binary mixtures with an uncertainty less than $\pm 0.5\%$.

In this work, it is reported experimental isothermal P-x-y data for the ternary system ETBE-cyclohexane-toluene and the binary systems involved at 313.15 K. Data reduction by Barker's method provides correlations for GE, using five-parameters Margules equation for the binary systems and the Wohl expansion for the ternary. Wilson, NRTL and UNIQUAC models have been applied successfully to both the binary and the ternary systems presented here. Excess enthalpies of the three binary mixtures have been determined at 298.15K and 313.15 K. The data have been correlated by the Redlich-Kister equation and NRTL model.

[1] J. J. Segovia, M. C. Martín, C. R. Chamorro, and M A Villamañán, *Fluid Phase Equilib.* **133**, 163 (1997).