

Improving Thermodynamic Consistency Among Vapor Pressure, Heat of Vaporization, and Liquid and Ideal Gas Isobaric Heat Capacities through Multi-Property Optimization

Joseph Hogge^{C, S}, Vincent Wilding, Thomas Knotts, Richard Rowley, Neil Giles and Richard Messerly

Department of Chemical Engineering, Brigham Young University, Provo, UT, U.S.A.

hogge.joseph@gmail.com

Vapor pressure, heat of vaporization, liquid isobaric heat capacity, and ideal gas isobaric heat capacity can be measured for pure organic compounds between the triple point and critical point. Additionally, heat of vaporization is proportional to the derivative of vapor pressure with respect to temperature through the Clapeyron equation, and the difference of liquid and ideal gas heat capacities are proportional to the derivative of heat of vaporization with respect to temperature. These relationships and experimental data were compared for several compounds to interpolate and extrapolate available data and increase consistency amongst these properties. A methodology for assessing the thermodynamic consistency amongst data sets and optimizing the accepted property values has been developed so that this procedure can be applied to other compounds in the DIPPR 801 database for which there are fewer experimental data available. The process involves critically evaluating available experimental data and the correlations used to fit these temperature-dependent properties. Multi-property optimization includes weighting the various data values based on the accuracy of the data and on the perceived relative importance of the properties in process design. User-defined weighting systems will be established to provide optimization flexibility across these properties for future use of the DIPPR 801 database.