An Equation of State for the Thermodynamic Properties of 1-Propanol

Kehui Gao
Key Laboratory of Thermo-Fluid Science and Engineering, Xi’an Jiaotong University, Xi’an, Shaanxi, China

Eric Lemmon
Applied Chemicals and Materials Division, NIST, Boulder, CO, U.S.A.

Jiangtao Wu
Key Laboratory of Thermo-Fluid Science and Engineering, Xi’an Jiaotong University, Xi’an, Shaanxi, China
jtwu@mail.xjtu.edu.cn

1-Propanol (C3H7OH) is saturated monohydric alcohol in structure. It can be used as solvent in paint and cosmetic industry. It also is a basic organic reagent to synthesize propylamine applied to produce medicine and agricultural chemical, feed additives, synthetic perfumes and so on. Recently, alcohols have attracted more and more attention as gasoline additives to reduce the formation of soot in combustion and cosolvent in the mixture with CO2 because of the high solubility of CO2 in them. However, there is no special equation of state for the thermodynamic properties of 1-propanol so far. In this work, on the basis of thermodynamic properties data from the literatures, a special Helmholtz Equation of State for 1-propanol was developed by the nonlinear fitting algorithm based on the Levenberg-Marquardt algorithm. It is explicit in Helmholtz energy with independent variables of temperature and density. The Equation of State is valid from the triple point temperature to 570K, for pressures up to 208MPa and for densities up to 17mol/dm³. The estimated uncertainties of properties calculated with the new equation in density, vapor pressure, saturated liquid density, saturated vapor density, and the properties with energy were evaluated. The behaviors of the equation of state were also assessed within the region of validity and at higher temperatures and pressures.