

Saturated and Compressed Liquid Heat Capacity at Constant Volume for 1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide

Nikolai Polikhronidi and Rabiyat Batyrova

Russian Academy of Sciences, Institute of Physics, Makhachkala, Dagestan, Russia

Ilmutdin Abdulagatov^S and Joseph Magee^C

Applied Chemicals and Materials Division, NIST, Boulder, Colorado, U.S.A.

joe.magee@nist.gov

Jiangtao Wu

Key Laboratory of Thermo-Fluid Science and Engineering of MOE, Xi'an Jiaotong University, Xi'an, Shanxi, China

With the goal of developing a reference equation of state for ionic liquid (IL) 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide at conditions for one-phase liquid and for two-phase liquid + vapor equilibrium, isochoric heat capacities (C_v) were reported for the first time [1]. The substance studied is often abbreviated [C6mim][NTf2] and is the already well-studied IUPAC reference IL. Measurements were conducted over the temperature range from (330 to 480) K and pressures up to 20 MPa using a high-temperature, high-pressure, nearly constant-volume adiabatic calorimeter. As useful byproduct of the measurement, densities were reported as a function of temperature and pressure. Measurements were made along liquid isochores in the range between $1218 \text{ kg}\cdot\text{m}^{-3}$ and $1279 \text{ kg}\cdot\text{m}^{-3}$. Furthermore, measurements were concentrated near the liquid-gas phase transition curve in order to closely observe phase changes. The values of temperature at the liquid-gas phase transition curve for each measured isochore (phase transition parameters, ρ_s , T_s) were obtained by analysis of quasistatic thermograms (readings of reference quality thermometer, T - τ plot, where τ is elapsed time) and barograms (readings of pressure transducer, P - τ plot). The combined expanded uncertainties of the density, ρ , and isochoric heat capacity, C_v , measurements at a 95 % confidence level with a coverage factor of $k = 2$ are estimated to be 0.06 % and 2.0 %, respectively. The combined expanded uncertainty of the phase-transition temperature is 0.02 K. One-phase (C'_{v1}) and two-phase (C'_{v2}) liquid isochoric heat capacities at saturation and saturation liquid densities (ρ'_s) of IL ([C6mim][NTf2]) were measured. The measured values of saturated caloric (C'_{v1} , C'_{v2}) and saturated thermal (ρ_s , T_s) properties were used to derive thermodynamic properties including (C_p , C_s , W , K_T , ΔH_{vap} , $(\partial P/\partial T)'_v$, and $(\partial V/\partial T)'_p$) of [C6mim][NTf2] at saturated liquid conditions. In addition, the second temperature derivatives of the vapor pressure (d^2P_s/dT^2) and the chemical potential ($d^2\mu_s/dT^2$) at liquid + vapor conditions, and the second temperature derivative of pressure at compressed liquid conditions (d^2P/dT^2)_p were calculated directly from the measured one- and two-phase isochoric heat capacity data. Values of (d^2P_s/dT^2) and (d^2P/dT^2)_p derived from calorimetric measurements were compared with the values calculated from vapor-pressure equations and from an IUPAC reference equation of state for this substance.

References

[1] N.G. Polikhronidi, R.G. Batyrova, I.M. Abdulagatov, J.W. Magee and J.T. Wu, *Physics and Chemistry of Liquids* 52, 657-679 (2014).