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

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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 kg⋅m$^{-3}$ and 1279 kg⋅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 isochoke (phase transition parameters, $\rho_s$, $T_s$) were obtained by analysis of quasistatic thermograms (readings of reference quality thermometer, $T-\tau$ plot, where $\tau$ is elapsed time) and barograms (readings of pressure transducer, $P-\tau$ plot). The combined expanded uncertainties of the density, $\rho$, 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 ($\rho'_s$) of IL ([C6mim][NTf2]) were measured. The measured values of saturated caloric ($C'_{v1}$, $C'_{v2}$) and saturated thermal ($\rho_s$, $T_s$) properties were used to derive thermodynamic properties including ($C_p$, $C_v$, $W$, $K_T$, $\Delta H_{vap}$, $(\partial P/\partial T)'_{v}$, 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