

Heat Capacity and Derived Thermodynamic Properties for Ionic Liquid Precursors: 1-Methylimidazole and 1-Bromobutane

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1-Alkyl-3-methylimidazolium ionic liquids (ILs) $[C_n\text{mim}]\text{An}$ are the most studied members of the class of room-temperature ILs. Normally, these compounds are synthesized in two stages. The first stage is quaternization of 1-methylimidazole resulting in formation of 1-alkyl-3-methylimidazolium chlorides $[C_n\text{mim}]\text{Cl}$ or bromides $[C_n\text{mim}]\text{Br}$. The second stage is the metathesis reaction during which the halogenide-ion is exchanged by another anion. Optimization of IL synthesis technology assumes knowledge of thermodynamic properties of the ILs as well as the intermediates and precursors. Earlier, we have calorimetrically determined heat capacities and parameters of fusion and glass transition for $[C_n\text{mim}]\text{Br}$ ($n = 2, 3, 4$) and a series of different 1-alkyl-3-methylimidazolium ILs. In this work we present the results of calorimetric investigation of precursors for IL synthesis: 1-methylimidazole (MeIm) and 1-bromobutane (BuBr). The heat capacity of the studied compounds was measured in an adiabatic calorimeter over the temperature range of (5 to 370) K. Both of the compounds were found to form crystalline and liquid phases. The fusion enthalpies were determined to be $D_{\text{fus}}H(272.16\text{ K}) = 12.08 \pm 0.02\text{ kJ}\times\text{mol}^{-1}$ for MeIm and $D_{\text{fus}}H(160.87\text{ K}) = 9.117 \pm 0.004\text{ kJ}\times\text{mol}^{-1}$ for BuBr. From the experimental data, thermodynamic functions of these compounds in the condensed state in the temperature range of (0 to 370) K were calculated. Based on the results obtained in the present work and the literature data on vaporization enthalpy, saturated vapor pressure, second virial coefficient, and formation enthalpy, the thermodynamic properties of BuBr in the ideal-gas state were found in a range of temperatures of (195 to 370) K.