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Experimental and Theoretical Thermodynamic Study of Distillable Ionic Liquid 1,5-Diazabicyclo[4.3.0]non-5-enium Acetate

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Abstract

© 2016 American Chemical Society. A thermochemical study of the protic ionic liquid 1,5-diazabicyclo[4.3.0]non-5-enium acetate ([DBNH][OAc]), a prospective cellulose solvent considered for the Ioncell-F process, was carried out. The heat capacities of 1,5-diazabicyclo[4.3.0]non-5-ene (DBN) and [DBNH][OAc] were measured by differential scanning calorimetry (DSC) at 223-323 and 273-373 K temperature ranges, respectively. The enthalpies of fusion and synthesis reaction of [DBNH][OAc] were measured by DSC and reaction calorimetry, respectively. The gas-, liquid-, and solid-phase enthalpies of formation of [DBNH][OAc] and DBN were determined using calorimetric and computational methods. The enthalpy of vaporization of [DBNH][OAc] was estimated from the formation enthalpies. The activity coefficients at infinite dilution of 17 and the enthalpies of solution at infinite dilution of 25 organic solutes in [DBNH][OAc] were measured by gas chromatography and solution calorimetry methods, respectively. The obtained data will be used in the design and optimization of the Ioncell-F process.

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