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Thermodynamic Properties of N-Methyl-Substituted Ethane-1,2-diamines: Experimental and Computational Study

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Abstract

© 2016 American Chemical Society.Vapor pressures for four N-methyl-substituted ethane-1,--diamines were measured using the transpiration method. Enthalpies of vaporization were derived from the temperature dependence of the vapor pressures. Consistency of the experimental data was assessed and confirmed with group-additivity (GA) and quantum-chemical (QC) methods. Further confirmation of the results is provided through combined assessment with properties reported in the literature for the parent compound ethane-1,--diamine and a group of alkyl-substituted alkane-1,2-diamines. The effective application of modern QC methods in critical evaluation of enthalpies of vaporization and enthalpies of formation is demonstrated.

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