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Benchmark Thermochemistry of N-Methylaniline

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Abstract

© 2015 American Chemical Society. In this work, the standard molar enthalpy of formation in the gaseous state of highly pure N-methylaniline, $\delta_f H_m^\circ(\text{g}, 298.15 \text{ K}) = 90.9 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$, has been obtained from the calorimetrically measured energy of combustion converted into the enthalpy of formation, $\delta_f H_m^\circ(\text{liq}, 298.15 \text{ K}) = 35.9 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$, and from the molar enthalpy of vaporization, $\delta_{\text{lg}} H_m = 55.0 \pm 0.2 \text{ kJ}\cdot\text{mol}^{-1}$, derived from vapor pressure measurements by transpiration method. The enthalpy of formation of N-methylaniline calculated using the quantum chemical G4 method was in excellent agreement with the experimental value. The frequencies of normal vibrations were obtained from the experimental and calculated spectra. Thermodynamic properties of N-methylaniline in the ideal gas state were calculated from molecular and spectral data in the temperature range 100-1500 K.

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