Journal of Physical Chemistry A 2015 vol.119 N10, pages 2142-2152

Benchmark Thermochemistry of N-Methylaniline

Emel'yanenko V., Pimerzin A., Turovtsev V., Verevkin S.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 American Chemical Society. In this work, the standard molar enthalpy of formation in the gaseous state of highly pure N-methylaniline, δfHm° (g, 298.15 K) = 90.9 ± 2.1 kJ·mol^{-1}, has been obtained from the calorimetrically measured energy of combustion converted into the enthalpy of formation, δfHm° (liq, 298.15 K) = 35.9 ± 2.1 kJ·mol^{-1}, and from the molar enthalpy of vaporization, δlgHm = 55.0 ± 0.2 kJ·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.

http://dx.doi.org/10.1021/jp5129854