

The NIST Chemistry WebBook: A Chemical Data Resource on the Internet

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The NIST Chemistry WebBook (<http://webbook.nist.gov>) is an Internet site that provides access to chemical and physical property data compiled by NIST and outside contributors. The site was established in 1996 and has grown to encompass a wide variety of thermochemical, ion energetics, solubility and spectroscopic data. Thermochemical data available includes heats of formation, heats of phase transitions, and heat capacities. Thermochemical properties of many reactions that support heat of formation values are provided.

The data available from the site are generally compiled by researchers with significant relevant experience. Data generally include references to the primary literature, an indication of how measurements were obtained, and additional meta-data as deemed appropriate by the archivist.

The site also includes two special features. The first is a set of interactive physical property models that provide thermodynamic and transport property data for a number of industrially important fluids. The second item is a group-additivity based estimator for gas phase thermodynamic properties. This estimator provides details on all the increments and corrections used in computing the estimate, so users can see how the estimated values were obtained.

This talk will discuss the data and computational tools available from the site. Usage patterns and future plans for the site will also be discussed.