

The NIST Chemistry WebBook: Chemical Informatics Challenges

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The NIST Chemistry WebBook (<http://webbook.nist.gov>) is a web 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, physical, solubility, spectroscopic, and chromatographic data. Thermochemical data available from the site includes heats of formation, heats of phase transitions, and heat capacities. Thermochemical properties of many reactions that support heat of formation values are also provided. The site includes a set of interactive physical property models that provide thermodynamic and transport property data at user supplied conditions for a number of industrially important fluids. A group-additivity based estimator for gas phase thermodynamic properties is also available. This talk will briefly discuss the site, the data available, and special features of the site. The second part of the talk will discuss the chemical informatics challenges encountered in putting together a site of this nature. In particular, issues concerning chemical identification and the applications of the new IUPAC International Chemical Identifier will be discussed. This identifier provides a convenient tool for identifying chemical species along with their stereoisomers and isotopomers. The identifier provides archivists with a new tool for searching for data and checking database consistency.