

## **NIST/TRC Databases and Software Tools for Chemistry and Engineering**

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The NIST Thermodynamic Research Center (NIST/TRC) is one of the oldest data research centers in the United States. For over 65 years of its history, TRC has produced a number of the periodical compilations and electronic databases that have become a major source of recommended data for scientific research and industrial process design, for both pure materials and mixtures. The first software product implementing the dynamic data evaluation concept was developed – NIST ThermoData Engine (TDE). This concept requires the development of large electronic databases capable of storing essentially all 'raw' experimental data known to date with detailed descriptions of relevant metadata and uncertainties. The combination of these databases with expert software designed primarily to generate recommended data based on the available experimental data and their uncertainties leads to the possibility of producing data compilations automatically 'to order', forming a dynamic data infrastructure. Two versions of TDE will be demonstrated: Standard Reference Database 103a encompassing properties of the pure compounds only, and Standard Reference Database 103b generating critically evaluated data for pure compounds, binary mixtures, and chemical reactions. ILThermo (NIST Standard Reference Database 147) - a free web research tool - allows users worldwide to access an up-to-date data collection from the publications on experimental studies of thermodynamic and transport properties of ionic liquids as well as binary and ternary mixtures containing ionic liquids. Efficient and reliable data dissemination has been one of the drivers for the development of ThermoML - IUPAC XML-based standard format for data storage and exchange. NIST/TRC is currently partnering with five major journals to encourage authors to submit their data for validation as part of the publication process. As part of this cooperation, the Guided Data Capture software (GDC) has been developed guiding authors through the process of data submission. The functional features of the GDC as well as ThermoML archive publicly available from the NIST/TRC Web site will be demonstrated. Web Thermo Tables (WTT, NIST Standard Reference Subscription Database 2 – Lite Edition, NIST Standard Reference Subscription Database 3 – Professional Edition) is a Web version of the TRC Thermodynamic Tables continuously distributed in hard-copy form to thousands of customers in scientific and engineering communities for the last 65 years in two series NIST/TRC Thermodynamic Tables-Hydrocarbons and NIST/TRC Thermodynamic Tables-Non-Hydrocarbons. NIST/TRC Ideal Gas Database (NIST Standard Reference Database 88) provides information on the most important thermodynamic properties (heat capacities, entropies, enthalpies, Gibbs free energies and enthalpies and Gibbs free energies of formation) of organic and some other compounds in the ideal gas state. There is a total of more than 2000 compounds. NIST Gas Hydrate Database is currently being developed to provide free Web access to experimental thermophysical, structural and other properties of the gas hydrates and clathrates.