

NIST/TRC Databases and Software Tools for Chemistry and Engineering

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The NIST Thermodynamics Research Center (NIST/TRC) is one of the oldest data research centers in the United States. For over 70 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, ternary mixtures, and chemical reactions.

Web Thermo Tables (WTT, NIST Standard Reference Subscription Database 2 – Lite Edition, <http://www.nist.gov/srd/nistwebsub2.cfm> ; NIST Standard Reference Subscription Database 3 – Professional Edition, <http://www.nist.gov/srd/nistwebsub3.cfm>) is a Web application of the NIST ThermoData Engine for pure compounds, available to the customers on a subscription basis.

ThermoPlan (NIST Standard Reference Database 167, <http://www.nist.gov/srd/nist167.cfm>) is a web application that provides free and open access for the broader research community to the experimental planning utilities that are incorporated into NIST ThermoData Engine. It provides recommendations for the relative merit of a proposed measurement via assessment of the existing body of knowledge, including availability of experimental thermophysical property data, variable ranges studied, associated uncertainties, state of prediction methods, and parameters for deployment of prediction methods. This web application provides utilities for the assessment of specific property measurements for pure and binary chemical systems, the broader data needs of pure systems, and recommendations for binary mixture measurements that could extend the current UNIFAC model.

ILThermo (NIST Standard Reference Database 147, <http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix>) - 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.

NIST Gas Hydrate Database (NIST Standard Reference Database 156, <http://www.nist.gov/srd/nist156.cfm>) provides free Web access to experimental thermophysical, structural and other properties of the gas hydrates and clathrates.