

## 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 on thermophysical and thermochemical properties of pure compounds and mixtures that have become a major data source for scientific research and industrial process design. NIST ThermoData Engine (TDE) is curation software that combines algorithmically encoded critical analysis, a comprehensive set of thermophysical and thermochemical property values from the open literature and a range of prediction methodologies to generate a database of recommended values on demand. Two versions of TDE will be demonstrated: Standard Reference Database (SRD) 103a encompassing properties of the pure compounds only and SRD 103b generating critically evaluated data for pure compounds, binary mixtures, ternary mixtures, and chemical reactions. ILThermo (NIST SRD 147, <http://ilthermo.boulder.nist.gov/index.html>) is a free web application that provides access to experimental thermodynamic and transport properties of neat ionic liquids, as well as binary and ternary mixtures containing ionic liquids, including citation and uncertainty recommendations. NIST Gas Hydrate Database (NIST SRD 156, <http://gashydrates.nist.gov/>) is a free web application that provides access to experimental thermodynamic and transport properties of gas hydrates and similar clathrates, including citation and uncertainty recommendations. ThermoPlan (NIST SRD 167, <http://trc.nist.gov/thermoplan/>) is a web application that provides free and open access to the experimental planning utilities powered by TDE. It provides assessment for the merit of a proposed measurement for pure compound or a mixture via assessment of the existing body of knowledge. ThermoLit (NIST SRD 171, <http://trc.nist.gov/thermolit/>) is a web application that provides free and open access to the literature search capabilities powered by TDE. It reports relevant literature citations and ranges of measurements for pure compound or mixture properties via assessment of the existing body of knowledge. Web Thermo Tables (WTT, Lite Edition - NIST SRD 202, <http://wtt-lite.nist.gov/> and Professional Edition - SRD 203, <http://wtt-pro.nist.gov/>) is a successor of TRC Tables and a web interface for TDE for pure compounds, available to the customers on a subscription basis.