

NIST ThermoData Engine version 10.4.2

Vladimir Diky, Ala Bazyleva^{C,5}, Eugene Paulechka, Joseph W. Magee, Andrei F. Kazakov, Demian Riccardi, Eric W. Lemmon and Ian H. Bell
Applied Chemicals and Materials Division, NIST, Boulder, CO, U.S.A.
ala.bazyleva@nist.gov

ThermoData Engine (TDE) developed by the NIST Thermodynamics Research Center is software for validation, analysis, and modeling of thermophysical and thermochemical properties for pure compounds and mixtures needed by chemical engineers and researchers. Depending on user's needs, TDE can provide a variety of functions at different levels of sophistication. Traditional functions include access to raw experimental data and automated property data evaluation involving literature (from the property database) and/or user's experimental data as well as predictions if necessary. The built-in database contains more than 7.5 million primary experimental property data values and is constantly amended with newly published and historical data as well as continuous data quality assessment with the use of additional information and methods. In addition to a larger database of experimental data and over 2000 enthalpies of formation from high-level quantum-chemical calculations, the present version provides improved implementation of its functions, also includes checking thermodynamic consistency of different properties, analysis of trends in compound series, comparison of models, validation of user's models (equations), and expert-mode refinement of models and special property calculations. New features currently under testing are stepwise evaluation, additional models and equations, and wider comparison capabilities.