

New Process for Delivery of Experimental Thermophysical and Thermochemical Property Data

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In order to establish a data depository system populated with the experimental thermophysical and thermochemical property data published in the Journal of Chemical and Engineering Data, procedures for direct data submission by the authors and subsequent unrestricted dissemination have been developed in cooperation among the Journal, NIST Thermodynamics Research Center (NIST/TRC), and DIPPR 991 Project.

The experimental data including numerical data, uncertainty estimates, and metadata descriptions are captured by Guided Data Capture software (GDC) with a strictly hierarchical system based upon rigorous application of the thermodynamic constraints of the Gibbs phase rule with full traceability to source documents. This software is freely available for download from the Internet. Following the peer-review process, authors are requested by the journal editors to download and use the GDC software to capture the experimental data that have been accepted for publication. The output of the GDC software is a batch data capture file, which is submitted directly to NIST/TRC. After additional consistency tests at the NIST/TRC Data Entry Facility, the files are converted into XML-based format (ThermoML) with software (TransThermo) developed at NIST/TRC. Upon release of the manuscript for publication, ThermoML files are posted on the NIST/TRC Web site for unrestricted public access. The developed process covers more than 120 properties of pure compounds, mixtures, and chemical reactions. Collected data will be downloaded into the relational database currently under development to provide users with various options for implementing data search mechanisms.