

## **Predictive Thermodynamics for Condensed Phases**

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## Supplementary Information

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**Physical and Chemical Data Sources for Thermodynamic and  
Thermochemical Properties**

***Journal of Physical and Chemical Reference Data.***

This journal, published jointly by the National Institute of Standards and Technology and the American Institute of Physics, contains contributions from the National Standard Reference Data System (NSRDS). It is used to provide critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation. Cumulative indexes are included periodically in the journals and University of Chicago authorized users have searchable access to contents and abstracts (1975-present) and full-text articles (2000-present) on the web. Articles too lengthy for regular issue publication are produced as *Monographs* and *Supplements*.

<http://ojps.aip.org/jpcrd/>

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***Thermochemical Data of Pure Substances.*** Ihsan Barin. 3rd edition. 2 volumes  
VCH: New York, 1995.

Covering about 230 organic substances in 2518 tables, functions include temperature dependent properties, heat capacity, entropy, Gibbs energy function, enthalpy, etc. Includes references and background information.

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***Thermodynamics of Organic Compounds in the Gas State.*** M. L. Frenkel. 2 volumes  
+ computer disk Thermodynamics Research Center: College Station, 1994.

Numerical data on heat capacity, entropy, enthalpy, Gibbs free energy for elements, inorganic compounds and C1 to C36 organics and organic radicals. Formula, name and CAS registry number indexes available.

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***Thermodynamic Properties of Individual Substances.*** L. V. Gurvich, I. V. Veyts and C. B. Alcock. 4th edition. 5 volumes (each in 2 pts) Hemisphere Publishing Co.: New York, 1989.

First published in 1956, under a slightly different title and under the auspices of the USSR National Standard Reference Data Service. Covers about 1100 condensed phase and gaseous substances comprised of 50 elements. Introduction contains a very good comparison of various data compilation handbooks. Each volume includes a textual and a tabular part and reports quantities like heat capacity, Gibbs energy, enthalpy, entropy, equilibrium constants for atomization of gases, sublimation or vapor equilibrium constants for condensed phases, and more. Values are reported up to a maximum of 20,000 degree Kelvin.

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***NIST-JANAF Thermochemical Tables.*** Jr. M.W. Chase. 4th edition. 2 volumes  
*Journal of Physical and Chemical Reference Data, Monograph 9 (1998)* American  
Chemical Society, American Institute of Physics: Washington, DC, 1998.

Recommended temperature-dependent values are provided for chemical thermodynamic properties of inorganic substances and for organic substances containing only one or two carbon atoms. These tables cover the thermodynamic properties over a wide temperature range with single-phase and multiphase tables for the crystal, liquid, and ideal gas state. The properties tabulated are heat capacity, enthalpy, entropy, Gibbs energy function, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states. All values are given in SI units and are for a standard-state pressure of 100 000 Pa (1 bar). Each tabulation is accompanied by a critical evaluation of the literature upon which the thermochemical table is based. Literature references are given. This volume is an update to the Third Edition which was published in *J. Phys. Chem. Ref. Data*, Volume 14 Supplement 1 (1985). It contains new and revised tabulations, In addition, it contains numerous corrections to errors (both typographical and numerical) which resulted from the massive changes made for the Third Edition.

NIST-JANAF Thermochemical Tables, Fourth Edition, Monograph No. 9 (Part I and Part II) is available from the American Institute of Physics, Suite 1NO1, 2 Huntington Quadrangle, Melville, NY 11747-4502.

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*NIST Standard Reference Database 85*

## **NIST/TRC Table Database**

This database, known as WinTable, is designed to retrieve and display recommended property values of pure compounds and is essentially the electronic version of the TRC Tables-Hydrocarbons and the TRC Tables-Non-Hydrocarbons which have been compiled by the Thermodynamics Research Center (TRC) for more than 50 years. At present, WinTable includes more than 497,000 property data points and 4,450 sets of equation coefficients for 7,468 compounds and 33 properties.

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WinTable contains the best available values of physical and thermodynamic properties of chemical compounds from the TRC Thermodynamic Tables - Non-hydrocarbons (critically evaluated data on the physical and thermodynamic properties of simple inorganic substances and organic compounds containing heteroatoms).

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**Key words:** thermodynamics, thermophysics, recommended data, critically evaluated data, thermophysical properties, TRC, Thermodynamics Research Center

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***Thermophysical Properties of Matter.*** Purdue University. Thermophysical Properties Research Center. 14 volumes IFI/Plenum: New York, 1970-1979.

Properties covered include thermal conductivity, specific heat, thermal radiative processes, thermal diffusivity, viscosity, and thermal expansion. Includes a master index.

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***TRC Thermodynamics Tables. Hydrocarbons.*** Thermodynamics Research Center. Multi-volume Texas A&M University: College Station, Produced by the Texas A&M University based Thermodynamics Research Center, this looseleaf collection is current

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***National Standard Reference Data Series (NSRDS-NBS).*** United States. National Bureau of Standards. 69 volumes Government Printing Office: Washington, DC, Formerly a companion publication to the *Journal of Physical and Chemical Reference Data*. This series generally included compilations that were very large, part of a



continuing series or based on a system, rather than a single property.

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***NBS Tables of Chemical Thermodynamic Properties, Selected Values of Inorganic and C1 and C2 Organic Substances in SI Units.*** Donald Wagman. American Chemical Society and American Institute of Physics: New York, 1982.

Provides enthalpies, free energies of formation, entropies and heat capacities for elements, inorganic compounds and organic compounds with one or two carbon atoms. Published as a supplement no. 2 to volume 11 of *Journal of Physical and Chemical Reference Data*.

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***Thermal Constants of Substances.*** Edited by V. P. Glushko, V. A. Medvedev, L. V. Gurvich and V. S. Yungman, Wiley: New York, 1999. Hard cover, 8 vols., 6592 pp., USD3700. **ISBN:** 0471318558

**Publisher's Note:**

Originally compiled in Moscow between 1965 and 1982, this renowned eight-volume set presents a comprehensive set of critically selected thermal constants of inorganic, simple organic, and metallo-organic substances. Featuring 25,976 substances and more than 51,500 references, the books cover a range of constants, including enthalpy and Gibbs energy formation, dissociation energy, enthalpy content, entropy and heat capacity at standard temperature, crystallographic and critical parameters, ionization potential, and electron affinity.

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