Thermo Data on the Web

Thermodynamic databases were once piles of books but are now accessible online.

Stephen R. Heller

Even if you passed physical chemistry as an undergraduate, you may well have struggled with obtaining data such as Gibbs free energy, entropy, and enthalpy for thermodynamic equations. For years, those who needed these values had no choice but to look them up in one of the numerous chemical data handbooks. Today, there is a better place to find thermodynamic data: the Web. Dozens of sources of thermo data are available on the Web. The University of Illinois at Chicago has an excellent webpage with links to over 100 data and property calculation websites (*http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property_html*). This article will cover just a few of the major sites, both free and paid, that are now available. These sites include the NIST Chemistry WebBook (*http://webbook.nist.gov*), DIPPR (*www.aiche.org/dippr*), DECHEMA (*www.dechema.de/f-infsys-e.htm*), and FIZ-Berlin Infotherm (*www.fiz-chemie.de/infotherm/servlet/infothermSearch*).

According to the National Institute of Standards and Technology (NIST), usage of the WebBook database and search system exceeds 20,000 users per week, with over 600,000 different IP addresses per year accessing just the WebBook. Although the WebBook covers a wide variety of subjects, its core is thermochemical and thermophysical data.

What are people doing with this information? In the chemical process industry, it would be difficult to build an efficient and cost-effective plant for producing a chemical without good, high-quality thermophysical and thermochemical properties. In the field of petroleum and bulk chemicals, where profit margins are slim, good data can be the difference between a well-run, profitable operation and one in the red. This information is needed for scale-up testing of large batches of chemicals. Thermodynamics data are used to design systems to minimize heat losses. They also help in the design of distillation columns. In these times, when everyone is cost-sensitive, good thermo data will improve both the quality of production and the quality of the product, leading to better profit margins.

Antoine Equation Parameters

$\log_{10}(P) = A - (B / (T + C))$
P = vapor pressure (bar)
T = temperature (K)

View plot Requires a Java capable browser.

Temperature (K)	A	B	C	Reference	Comment
369. - 522.3	4.47834	1771.357	-127.484	Stull, 1947	Coefficents calculated by NIST from author's data.

Figure 1. NIST WebBook Antoine equation data for benzoic acid. (Courtesy of NIST.)

NIST Chemistry WebBook

The Chemistry WebBook is by far the most used source of thermodynamics data. At present, all the information in the WebBook is free, which, in addition to the high quality of the evaluated data, is probably the major reason for its high and widespread use. It contains data on over 48,000 chemicals, including thermochemical data for more than 7000 organic and small inorganic compounds, such as enthalpy of formation, enthalpy of combustion, heat capacity, entropy, phase transition enthalpies and temperatures, and vapor pressure. In addition, there are reaction thermochemistry data for over 8000 reactions on enthalpy of reaction and free energy of reaction.

The WebBook has numerous easy-to-use search capabilities, including chemical name, formula, molecular weight, CAS Registry Number, author, structure, substructure, and reaction.

DIPPR

The Design Institute for Physical Properties (DIPPR) is a part of the American Institute of Chemical Engineers. With funding from the chemical industry, DIPPR has undertaken 7 major projects over the past 2 decades, and one of them, a database of 1743 chemicals, has become the industry standard for the physical properties of pure components.

The DIPPR database consists of experimental data, estimated values where necessary, temperature-dependent correlation coefficients, references, notes, quality codes, and other information required for proper use of the DIPPR database in computer-accessible form, together with software for searching, accessing, and using the data and accompanying information.

The database also includes source data values and references, data quality codes, and background information, such as molecular structure, synonyms, hazard properties, miscellaneous properties, notes, and explanations. It now contains data for 29 fixed-value properties and 15 temperature-dependent properties. When the project is completed, data for approximately 1811 industrially important compounds will be included. As far as possible, values of all these properties are entered for each chemical. If experimental data are not available, values are esti-

KEY TERMS: data handling, materials/nanotech

Search results: 5 hits page 1 /1

Lines		USD	property description	substance/mixture	year	temperature	pressure
☐	1	13.47	Antoine equation log(p) = A - B/(C+T), T= 150 ... 479 Celsius	benzoic acid	1995	-	-
☐	1	13.47	Antoine constant	benzoic acid	1989	-	-
☐	1	13.47	Antoine-constants log(p/Torr) = A - B/ ((T/deg C)+C)	benzoic acid	1983-2002	-	-
☐	3	28.06	Coefficients of the Antoine vapor pressure equation	benzoic acid	1979	-	-
☐	1	13.47	Antoine constant,boiling temperature	benzoic acid	1976	-	-

Figure 2. DECHEMA Antoine equation data for benzoic acid. (Courtesy of DECHEMA.)

mated when possible. Temperature-dependent correlation coefficients, applicable upper and lower temperature limits, and values computed at these limits are included for temperature-dependent properties. Fundamental SI units are used.

The DIPPR database is available online via the Chemical Abstracts Service STN computer network (*www.cas.org*). It is also available in a limited form at Brigham Young University (BYU). If you are a student or employee of an educational institution and would like access to the DIPPR 801 student database, go to *http://dippr.byu.edu/students/chemsearch.asp*.

DECHEMA

The Society for Chemical Engineering and Biotechnology (DECHEMA) is a nonprofit scientific and technical society based in Frankfurt/Main, Germany. It was founded in 1926. One of its main activities has been the creation and dissemination of the DETHERM database and search system.

The DETHERM database provides thermophysical property data for about 21,000 pure compounds and 101,000 mixtures. These data are indispensable for the design of apparatus and chemical production facilities.

DETHERM contains literature values together with bibliographical information, descriptors, and abstracts. At this writing, 4.2 million data sets are stored that contain the following properties: phase equilibrium data, vapor pressures, critical data, thermodynamic properties, transport properties, surface tensions, and electrolyte data.

Infotherm—FIZ-Berlin

The last database and search system to be described here is the Infotherm system from FIZ-Berlin—the Chemistry Information Centre (Fachinformationszentrum Chemie, FIZ Chemie Berlin). Launched in late 2003, the Infotherm database of the thermophysical properties of substances is written in Extensible Markup Language (XML), allowing both human users and computers to read and understand the information. By making Infotherm available via the Web, FIZ Chemie Berlin hopes to target those chemical engineering offices and companies that are increasingly using the Internet to meet their information requirements. The integration of the database in company intranets is simple using XML technology.

The high-quality Infotherm database delivers data on pure compounds and on mixtures, such as pressure-volume-temperature (PVT) properties, phase equilibria, transport and surface properties, calorific properties, and solid–liquid equilibria. The complete database contains more than 90,000 data records for mixtures and about 199,000 for pure substances. The first release in late 2003 contained more than 80,000 data sets on mixtures and more than 60,000 on pure compounds. Each piece of data may be accessed via the chemical name, trivial name, molecular formula, or CAS Registry Number. The data originate from journal articles, handbooks, and data collections that are evaluated by FIZ Chemie Berlin and cover the period from 1985 until the present. The database is updated monthly. It provides information on the thermophysical properties of 6300 pure chemical compounds and 23,000 mixtures, along with full bibliographic data. Some 150,000 tables contain PVT properties, phase equilibria, transport and surface properties, calorific properties, and acoustic and optical properties.

Searching the database and the "preview" display format of results is free of charge. This policy is somewhere between the search policy for the NIST data, which are available at no cost, and

Infotherm result

FIZ CHEMIE BERLIN Fachinformationszentrum Chemie GmbH

infotherm | login | logout | my infotherm | help

Hello **Mr. steve heller** session cost: 0 € amount spent: 0 €

result previous < 1 > next hits: 1-1 / 1

contract
free access
select

system: Benzoic acid 1/1
properties: Antoine constant A, Antoine constant B, Antoine constant C, temperature, temperature lines: 1
title: Liquid-vapor equilibrium in systems containing semi-products of the synthesis of benzoic acid. Part 4
author(s): Abramov, V. E.; Smirnova, N. A.
conditions: vapor-liquid equilibrium, saturated condition

property	min	max	unit	value type
Antoine constant A	xx.xx	xx.xx	-	by regression
Antoine constant B	xx.xx	xx.xx	-	by regression
Antoine constant C	xx.xx	xx.xx	-	by regression
temperature	458	524	K	preset
temperature	458	524	K	preset

Figure 3. Infotherm Antoine equation data: complete output for benzoic acid. (Courtesy of FIZ-Berlin.)

the DECHEMA data, which are all for a fee. The website does let you know when the information is available at no cost. Infotherm offers pay-per-view access or full access to all documents on a license basis. Pay-per-view users can purchase full access to an individual document from the free-preview format. For considerable flexibility, all purchased documents can be downloaded in several data formats. (Note: The CSV (comma-separated value) download exports only the data in a spreadsheet format, such as MS Excel.) Optionally, the user can store all documents in the "my infotherm" section by selecting from the hit list. These documents will be available in future sessions. Besides licensing the entire database, customers can purchase prepaid packages, which can be transformed into an unlimited license if the usage exceeds the respective license fee.

Antoine Equation Data

An example of a search in three of these systems and the resulting outputs is shown in Figures 1–3. In the examples, the search was for Antoine equation data for benzoic acid to estimate the vapor pressure at different temperatures.

Chemists often use the Clausius–Clapeyron equation to estimate the vapor pressure of pure liquids or solids, and it works well for most applications. Several of the assumptions made in the derivation of the equation fail at high pressure and near the critical point, giving inaccurate results. Chemical engineers often need more reliable vapor pressure estimates. The Antoine equation is a simple three-parameter fit to experimental vapor pressures measured over a restricted temperature range:

$$\log P = A - \frac{B}{T + C}$$

where A, B, and C are Antoine coefficients that vary from substance to substance. Sublimations and vaporizations of the same substance have separate sets of Antoine coefficients, as do components in mixtures. The Antoine equation is accurate to a few percent for most volatile substances (with vapor pressures over 10 Torr).

The NIST WebBook results are shown in Figure 1, and all data from the DECHEMA database are available for a fee, which is shown in each of the five hits in Figure 2.

The search in the Infotherm system starts out with the webpage displaying the search options, including search by name; formula; CAS Registry Number; type of data you want to search for (the pulldown menus list dozens of properties, as in the DECHEMA search system); a bibliography search for author, title, and so on; and type of system (pure, binary, and then up to denary).

Figure 3 shows the detailed output from Infotherm. This example is from a record that is available at no cost.

In summary, thermodynamics data, an important need for industrial research, is now widely available via the Web. The examples shown here are just a few of the many sources of this information and again prove why the Web is such a wonderful resource in making it easier for today's chemists to do their work quickly and efficiently.

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