NIST Standard Reference Database 88

NIST/TRC Ideal Gas Database
Version 2.0

Users' Guide

Data compiled and evaluated by:

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TABLE OF CONTENTS

1. INTRODUCTION

1.1 Database Description

The NIST TRC Ideal Gas database (TRCIGD) provides information on the most important thermodynamic properties (heat capacities, entropies, enthalpies, Gibbs free energies and enthalpies and Gibbs free energies of formation) of organic (and some other) compounds in the ideal gas state. The database contains a total of more than 2000 compounds. The heat capacities are calculated using coefficients of linear or non-linear functions of their temperature dependence. These coefficients were obtained based on the results of statistical mechanical or additive calculations. The other properties (entropies, enthalpies and Gibbs free energies) are determined by integration using a heat capacity function. The enthalpies and Gibbs free energies of formation are calculated based on the properties of the individual compounds and the properties of their elements in the standard states. The calculations can be performed in two different regimes: NON-LINEAR and POLYNOMIAL. The regime POLYNOMIAL uses a linear function to represent temperature dependence of heat capacity. This function is simple and commonly used in engineering applications. However, there may not be a sufficient number of significant digits to insure sufficient accuracy at temperatures higher than 3000 K. When choosing the NON-LINEAR regime, the heat capacities are calculated using the non-linear function of temperature. This function is quite complicated, but it ensures sufficient accuracy over a wide temperature range. The NON-LINEAR regime is the default selection when the user starts running this database. The new version 2.0 is run by new window interface.

1.2 Installation

To install the NIST TRC Ideal Gas Database (TRCIGD) on your hard drive, insert the CD-Rom, go to Start/Run and click on the program setup.exe.

1.3 System Requirements:

The program requires Pentium processor, [®]Windows 2000 or XP, and at least 64 Mb memory (256 recommended).

2. Use of the Program

2.1 Selection of Compounds

Multiple compounds can be selected and accumulated in a list. To add a compound, CLICK the "Add compound" button and enter any combination of formula (partial formula) and name (partial name) on the compound selection form.

(1) Enter Empirical Formula and/or Name:
  (A) Empirical Formula
      0Enter the entire empirical formula
      1(e.g., C5H5N, (NH2)2CO)
  (B) Name
      0Enter the entire name or use wildcards (*)
      1(e.g., 2-methylpyridine, 2-methylp*, 2-*-pyridine)

(2) CLICK "Find" to complete the search
  (A) If the compound appears in the list
      0Select the compound from the list and
      1CLICK "Accept"

(3) Repeat (1)-(2) to add another compound or CLICK "Done"

  NOTE: Symbols for elements are case sensitive (e.g., use "Br" and not "BR" or "br" for bromine)

  Compounds can be removed from the list by pressing the Delete key. The compound list can be cleared by clicking the "Clear compounds" button.

2.2 Selection of Temperatures

Selected temperatures are accumulated in a list. To add temperatures, CLICK the Add temperature button and enter temperatures separated by spaces and/or a temperature range specified by the lower temperature, higher temperature, and temperature step on the temperature-selection form.

Temperatures can be removed from the list by pressing the Delete key. The temperature list can be cleared by clicking the "Clear T" button.

2.3 Selection of Equations

To complete the request, CLICK either the "Get data (linear equation)" or "Get data (non-linear equation)" button.

The mathematical forms of the equations are given later in this Help.

2.4 Saving the Data

The data can be saved in a file through the menu File->Save or by pressing the Ctrl-S key combination. Otherwise, all or any part of the results can be highlighted and copied to the system clipboard by pressing Ctrl-C.

3. Output Specifications

The output consists of 7 columns; the last two are present if the enthalpy of formation is available.

T (K)	Temperature
C_p (J/K/mol)	Heat capacity at constant pressure
S (J/K/mol)	Absolute entropy
(H-H0)/T (J/K/mol)	Reduced enthalpy (divided by temperature); reference state is ideal gas at T = 0 K
-(G-H0)/T (J/K/mol)	Negative reduced Gibbs energy (divided by temperature); reference state is ideal gas at T = 0 K
H_{Form} (kJ/mol)	Enthalpy of formation
G_{Form} (kJ/mol)	Gibbs energy of formation

NOTE: All values correspond to 1 bar pressure.

Parameters $α_i$, I, J of smoothing equations used to generate the tabulated data along with their ranges of validity are also included in the output. The equations are described later in this Help.

UNCERTAINTIES. As traditionally published, the values of the calculated heat capacities, entropies, reduced enthalpies, and reduced Gibbs energies are represented with two decimal places while enthalpies and Gibbs energies of formation are displayed with one decimal place. The uncertainties of the calculated thermodynamic functions are estimated to be around 1% . This estimate does not include the uncertainties related to the contributions associated with the selection of the models for anharmonicity, existence of the tautomers and conformers as well as complex internal rotations.

NIST/TRC 3

4. SMOOTHING EQUATIONS

Two smoothing equations are used in this database to represent ideal-gas heat capacities and derived properties as functions of temperature, linear and non-linear. You can choose one of them at a time. Linear equation works in a restricted temperature range, usually below or above 1000 K, so generally two linear equations smoothly connecting at certain temperature are provided for each compound in the database. Non-linear equation covers the whole temperature range for a compound.

4.1 Linear equation

$$C_p^0 / R = \sum_{i=0}^{4} a_i T^i$$

$$\frac{H^0(T) - H^0(0)}{RT} = I/T + \sum_{i=0}^{4} \frac{1}{1+i} a_i T^i$$

$$S^0(T)/R = J + a_0 \cdot \ln(T) + \sum_{i=1}^{4} \frac{1}{i} a_i T^i$$

where

C_p^0 ideal-gas heat capacity
$(H^0(T) - H^0(0))$ enthalpy (reference state is ideal gas at $T = 0$ K)
$S^0(T)$ absolute entropy at temperature T and $P^0 = 1$ bar
R gas constant
T temperature
a_i, I, J equation parameters

4.2 Non-linear equation

$$C_p^0 / R = a_0 + (a_1/T)^2 \cdot x(a_2) + a_3 \cdot y^2 + (a_4 - a_5/(T-a_7)^2) \cdot y^8$$

with

NIST/TRC 4

$$y = \frac{T - a_7}{T + a_6}$$
if $T > a_7$; 0 if $T \le a_7$

$$x(a_2) = \exp(-a_2 / T)$$

$$\frac{H^0(T) - H^0(0)}{RT} = a_0 + a_1 x(a_2) f(a_2, T) + I/T + h(T)/T$$

with

$$h(T) = (2a_3 + 8a_4)\ln(1-y) + \left\{ a_3\left(1 + \frac{1}{1-y}\right) + a_4\left(7 + \frac{1}{1-y}\right) \right\} y + a_5\left(3y^2 + \frac{5}{3}y^3 + y^4 + \frac{3}{5}y^5 + \frac{1}{3}y^6\right) + \frac{1}{7}\left\{ a_6 - \frac{a_3}{(a_6 + a_7)^2} \right\} y^7$$

if $T > a_7$; 0 if $T \le a_7$

$$S^0(T)/R = J + a_0 \cdot \ln(T) + \frac{a_1}{a_2^2}\left(1 + \frac{a_2}{T}\right)x(a_2) + s(T)$$

with

$$s(T) = \left\{ a_3 + \left(\frac{a_4 a_7^2 - a_5}{a_7^2}\right)\left(\frac{a_7}{a_6}\right)^i \right\}\left(\frac{a_7}{a_6}\right)^3 \ln(z) + (a_3 + a_4)\ln\left(\frac{T + a_6}{a_6 + a_7}\right) + \sum_{i=1}^{i}\left\{ \left(\frac{a_4 a_7^2 - a_5}{a_7^2}\right)\left(\frac{-a_7}{a_6}\right)^{4-i} - a_4 \right\}\frac{y^i}{i} - \left\{ \frac{a_5(a_6 + a_7)}{a_6} + \frac{a_5 y^6}{7a_7(a_6 + a_7)} \right\} y$$

if $T > a_7$; 0 if $T \le a_7$

where

C_p^0 ideal-gas heat capacity
$(H^0(T) - H^0(0))$ enthalpy (reference state is ideal gas at T = 0 K)
$S^0(T)$ absolute entropy at temperature T and P^0 = 1 bar
R gas constant
T temperature
a_i, I, J equation parameters
The equations are also described in the literature:

Michael Frenkel, G.J.Kabo, K.N.Marsh, G.N.Roganov, and R.C.Wilhoit
Thermodynamics of Organic Compounds in the Gas State, Vol. 2
Thermodynamics Research Center: College Station, TX, 1994
ISBN 1-883400-04-X

Linear equation: Equation 3.34, Page 539.
Non-linear equation: Equation 3.30, Page 537.

5. References

Michael Frenkel, G.J.Kabo, K.N.Marsh, G.N.Roganov, and R.C.Wilhoit
Thermodynamics of Organic Compounds in the Gas State, Vol. 1 and 2
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ISBN 1-883400-05-8

NIST/TRC 6

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