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Thermo physical chemical properties of fluids using the free NIST chemistry web book database

Abstract

Many engineers, students, teachers, academicians, scientists, and researchers need to know intensive thermal, physical, and chemical properties of a fluid at a certain equilibrium state (as determined by temperature and pressure, for example). Such properties include the density, specific volume, viscosity, specific heat capacity, thermal conductivity, speed of sound, specific enthalpy, specific entropy, and surface tension. This article refers to a powerful database for such information, which is called NIST Chemistry Web Book. It is owned by the National Institute of Standards and Technology (NIST), which is an agency of the United States Department of Commerce. The database is available online free-of-charge and does not require registration for access. Its use is simple, and it offers the user multiple options for the unit to be used for each individual property. An application is presented where the density, dynamic viscosity, specific heat at constant pressure, and thermal conductivity for water at its liquid phase are presented at an absolute pressure of 1 bar over a temperature range from 1°C to 99°C. Comparisons with two sources support the correctness of the database.

Keywords: fluids, properties, thermal. physical, chemical, water

Volume 1 Issue 1 - 2017

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Received: May 20, 2017 | **Published:** August 28, 2017

Abbreviations: IR, infrared; UV, ultraviolet (visible); IUPAC, international union of pure and applied chemistry; InChI, international chemical identifier; InChIKey, new fixed-length code that represents a InChI; CAS, chemical abstracts service; NIST, national institute of standards and technology; SRD, standard reference data.

Introduction

Fluids (gases and liquids) are encountered heavily in different specializations of engineering and science. Engineers and researchers may frequently need an easy access to a reliable and rich database of fluid properties at a wide range of conditions during their work. Example uses are the design of plumbing systems, ventilation or air-conditioning systems, cooling cycles, and structures subject to wind loads, plasma flows, and various chemical processes. In teaching, the data in an appendix of a textbook might be sufficient to meet the need of a course. However, a much deeper and boarder database is needed to satisfy the scope of practical applications, especially with multidisciplinary nature. This work explores one such extensive database, showing how powerful it is. Being freely available online and well-documented increases its value. A specific example for using it is provided for liquid water as a sample fluid.

NIST chemistry web book

The National Institute of Standards and Technology (NIST) developed a program called Standard Reference Data (SRD),[1] which covers chemistry, engineering, fluids and condensed phases, material sciences, mathematics, computer sciences, and physics. One component of this program is called NIST Chemistry Web Book,[2] which is a rich database that offers several thermo-physical-chemical properties of fluids and other species.

The information in the database spans (as of July 29, 2017) the following categories:

A. Thermophysical property data for 74 fluids

i. Density, specific volume
ii. Heat capacity at constant pressure
iii. Heat capacity at constant volume
iv. Specific enthalpy
v. Specific internal energy
vi. Specific entropy
vii. Dynamic viscosity
viii. Thermal conductivity
ix. Joule-Thomson coefficient
x. Surface tension (saturation curve only)
xi. Speed of sound

B. Thermochemical data for over 7,000 organic and small inorganic compounds

i. Enthalpy of formation
ii. Enthalpy of combustion
iii. Heat capacity
iv. Entropy
v. Phase transition enthalpies and temperatures
vi. Vapor pressure
vii. Reaction Thermochemistry data for over 8,000 reactions
viii. Enthalpy of reaction
ix. Free energy of reaction
x. Ion Energetics data for over 16,000 compounds
xi. Ionization energy

xii. Appearance energy

xiii. Electron affinity

xiv. Proton affinity

xv. Gas basicity

xvi. Cluster ion binding energies

C. IR spectra for over 16,000 compounds

D. UV/Vis spectrum

E. Constants of diatomic molecules (spectroscopic data) for over 600 compounds

F. Gas chromatography data for over 27,000 compounds.[3–6]

The following fluids are among the ones in the NIST Chemistry Web Book database shown in Table 1. For fluids, some temperature-dependent properties can be displayed in a tabular form or as an interactive graph (which can be saved as a PNG image file shown in Figures 1–8. The database provides proper references that support the data presented for each fluid. One can specify the fluid (or the chemical species in general) by any of five methods as explained in Table 2, with the values of water being given as an example.

Table 1 List of fluids in NIST chemistry web book database

1	Water	31	Decane
2	Nitrogen	32	Dodecane
3	Hydrogen	33	Helium
4	Parahydrogen	34	Neon
5	Deuterium	35	Argon
6	Oxygen	36	Krypton
7	Fluorine	37	Xenon
8	Carbon monoxide	38	Ammonia
9	Carbon dioxide	39	Nitrogen trifluoride
10	Dinitrogen monoxide	40	Trichlorofluoromethane (R11)
11	Deuterium oxide	41	Dichlorodifluoromethane (R12)
12	Methanol	42	Chlorotrifluoromethane (R13)
13	Methane	43	Tetrafluoromethane (R14)
14	Ethane	44	Dichlorofluoromethane (R21)
15	Ethene	45	Methane, chlorodifluoro- (R22)
16	Propane	46	Trifluoromethane (R23)
17	Propene	47	Methane, difluoro- (R32)
18	Propyne	48	Fluoromethane (R41)
19	Cyclopropane	49	1,1,2-Trichloro-1,2,2-trifluoroethane (R113)
20	Butane	50	1,2-Dichloro-1,1,2,2-tetrafluoroethane (R114)
21	Isobutane	51	Chloropentafluoroethane (R115)
22	Pentane	52	Hexafluoroethane (R116)
23	2-Methylbutane	53	Ethane, 2,2-dichloro-1,1,1-trifluoro- (R123)
24	2,2-Dimethylpropane	54	Ethane, 1-chloro-1,2,2,2-tetrafluoro- (R124)
25	Hexane	55	Ethane, pentafluoro- (R125)
26	2-Methylpentane	56	Ethane, 1,1,1,2-tetrafluoro- (R134a)
27	Cyclohexane	57	1,1-Dichloro-1-fluoroethane (R141b)
28	Heptane	58	1-Chloro-1,1-difluoroethane (R142b)
29	Octane		
30	Nonane		

Table 2 The five methods to specify a fluid in NIST chemistry web book

Specification method of a fluid	Example for water
Name	Water
Chemical formula	H_2O
IUPAC [3] identifier string InChI[4]	$1S/H_2O/h1H_2$
IUPAC identifier string InChIKey[5]	XLYOFNOQVPJJNP-UHFFFAOYSA-N
CAS[6] registry number	7732-18-5

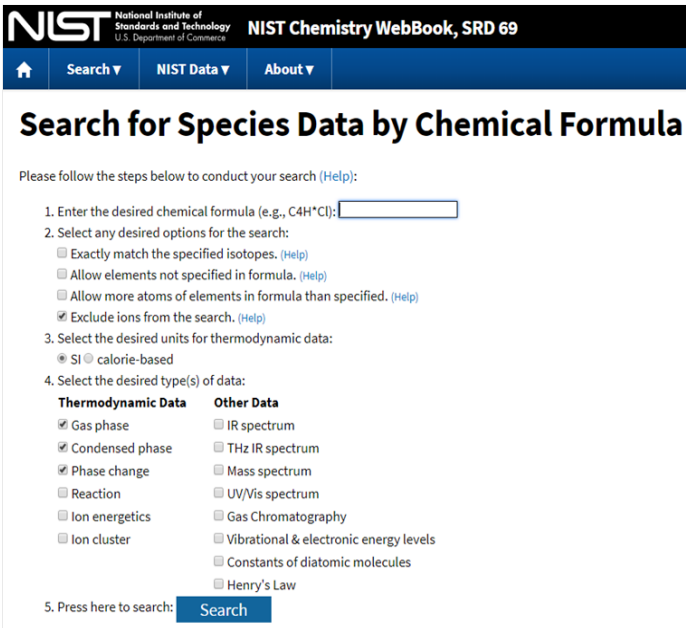

Figure 1 A snapshot of the online database (NIST Chemistry WebBook) when selecting a species by its chemical formula.

Some water properties

We consider here liquid-water as an example fluid and present the variation of four thermo physical properties that are commonly used in some engineering disciplines with temperature at a constant pressure of 1 bar (10^5Pa), which is approximately equal to one standard atmosphere (101,325 Pa). The temperature range is from 1°C to 99°C. The properties are:

a. Density (in kg/m^3)

Citation: Marzouk OA. Thermo physical chemical properties of fluids using the free NIST chemistry web book database. *Fluid Mech Res Int* . 2017;1(1):14–18. DOI: 10.15406/fmrij.2017.01.00003

b. Dynamic/Absolute viscosity (in centipoises, cP);

c. Specific heat at constant pressure (in J/g.°C)

d. Thermal conductivity (in W/m.°C)

e. Specific volume (in cm^3/g)

f. Kinematic viscosity (in centistokes, cSt)

g. Specific heat at constant volume (in J/g.°C)

h. Speed of sound (Inm/s)

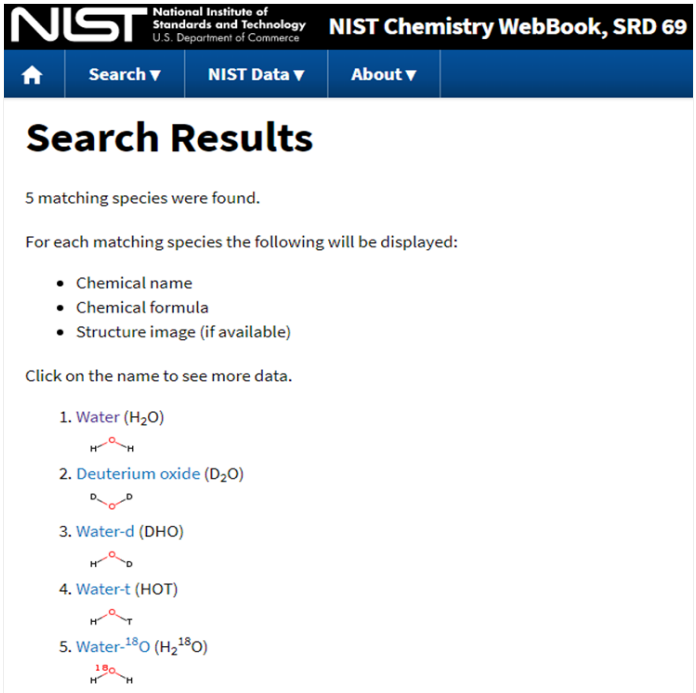

Figure 2 A snapshot of the online database (NIST Chemistry Web Book) showing the search results for the chemical formula, H_2O.

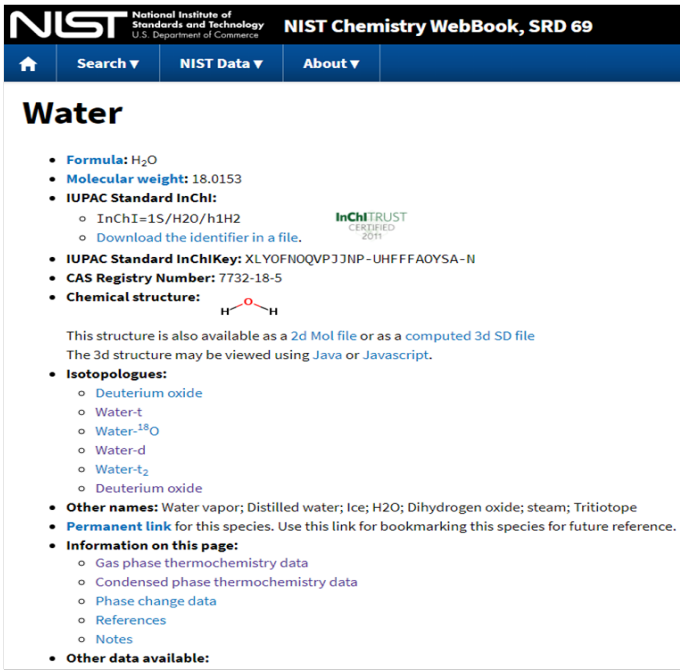

Figure 3 A snapshot of the online database (NIST Chemistry Web Book) after selecting water.

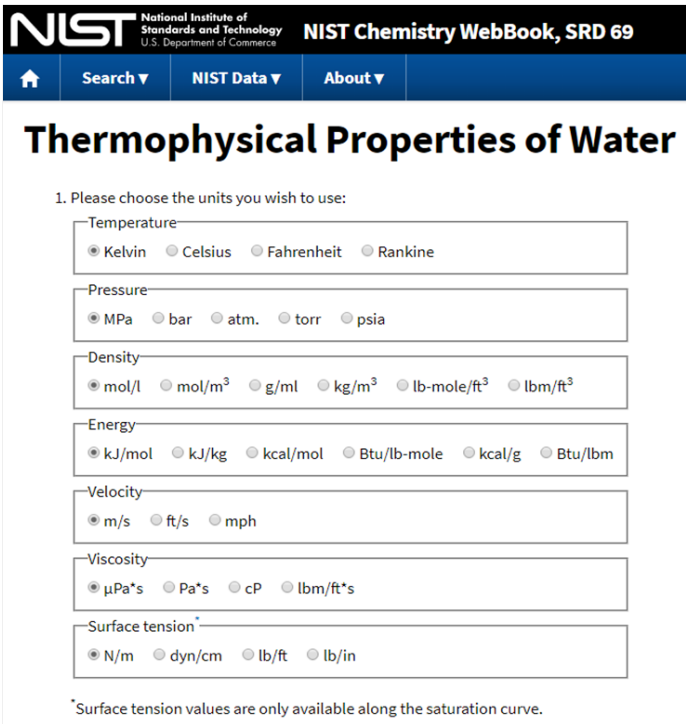

Figure 4 A snapshot of the online database (NIST Chemistry Web Book) when attempting to display the Fluid Properties of water.

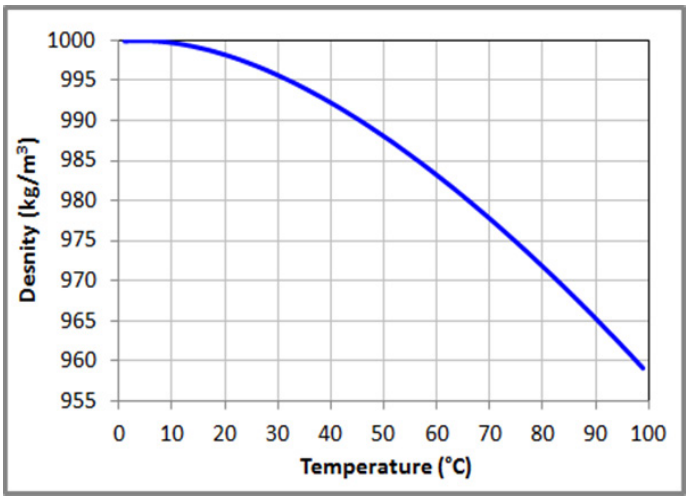

Figure 5 Variation of the density with temperature for liquid water at 1bar based on the data obtained from NIST Chemistry Web Book.

The following formulas provide conversions factors from other units used for the above properties to the ones used here:[7–9]

$$\frac{lb_m}{in^3} = 2.768 \times 10^4 \frac{kg}{m^3} \quad (1)$$

$$\frac{lb_m}{ft^3} = 16.02 \frac{kg}{m^3} \quad (2)$$

$$\frac{slug}{ft^3} = 515.4 \frac{kg}{m^3} \quad (3)$$

$$\frac{g}{cm^3} = 10^3 \frac{kg}{m^3} \quad (4)$$

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$$\frac{m^3}{kg} = 10^3 \frac{cm^3}{g} \quad (5)$$

$$Pa.s = 10^3\ cP \quad (6)$$

$$poise\left(\frac{dyn.s}{cm^2}\right) = 100\ cP \quad (7)$$

$$reyns\left(\frac{lb_f.s}{in^2}\right) = 6.895\ cP \quad (8)$$

$$\frac{mm^2}{s} = cSt \quad (9)$$

$$stokes\left(\frac{cm^2}{s}\right) = 100\ cSt \quad (10)$$

$$\frac{m^2}{s} = 10^6\ cSt \quad (11)$$

$$\frac{in^2}{s} = 645.2\ cSt \quad (12)$$

$$\frac{ft^2}{s} = 9.290 \times 10^4\ cSt \quad (13)$$

$$\frac{J}{kg.K} 10^3 \frac{J}{g.℃} \quad (14)$$

$$\frac{Btu}{lb_m.°F} = 4.187 \frac{J}{g.℃} \quad (15)$$

$$\frac{Btu}{hr.ft.°F} = 1.731 \frac{W}{m.℃} \quad (16)$$

$$\frac{km}{h} = \frac{1}{3.6}\frac{m}{s} = 0.2778\frac{m}{s} \quad (17)$$

$$\frac{ft}{s} = 0.3048\frac{m}{s} \quad (18)$$

$$\frac{mi}{h} = 0.44704\frac{m}{s} \quad (19)$$

Four of the above properties are related as following viscosities are related as:

$$specific\ volume = \frac{1}{density} \quad (20)$$

$$kinematic\ viscosity = \frac{dynamic\ viscosity}{density} \quad (21)$$

Validation

To judge the accuracy of the values in the NIST Chemistry Web Book, we compare selected values taken for the properties of water as taken from that database with those available in two other sources. The first source is appendix C in a classic reference in the area of water treatment.[10] The second source is a software package.[11] The comparisons are made at one standard atmospheric pressure (101,325 Pa) for the isobaric (constant-pressure) water data of density in Table 3 and for dynamic viscosity in Table 4. The fluid is water in both tables. The values taken from the NIST Chemistry Web Book database agree well (and sometimes are identical to) those taken from the other sources. This agreement suggests that the database was prepared carefully and can be used reliably.

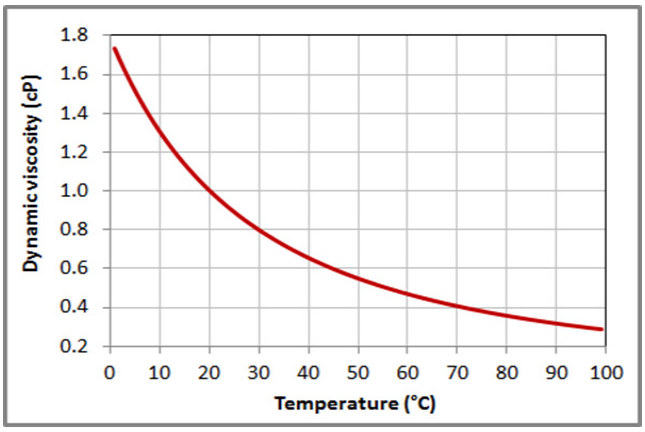

Figure 6 Variation of the dynamic viscosity with temperature for liquid water at 1bar based on the data obtained from NIST Chemistry Web Book.

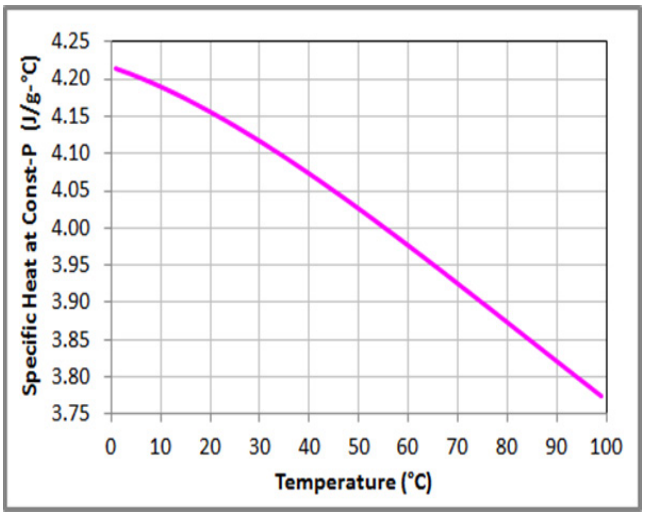

Figure 7 Variation of the specific heat capacity at constant pressure with temperature for liquid water at 1bar based on the data obtained from NIST Chemistry Web Book.

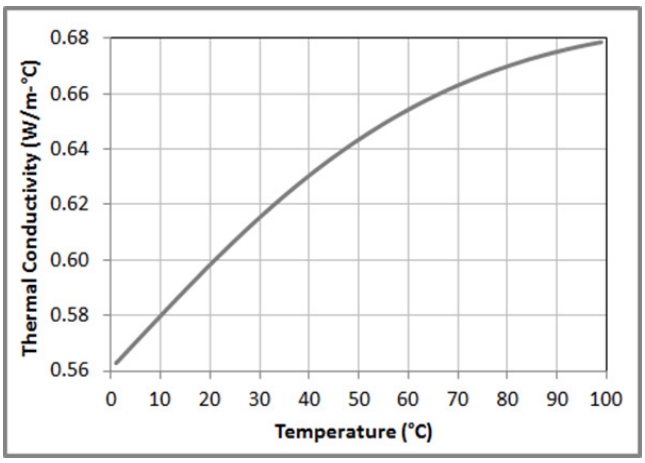

Figure 8 Variation of the thermal conductivity with temperature for liquid water at 1bar based on the data obtained from NIST Chemistry Web Book.

Citation: Marzouk OA. Thermo physical chemical properties of fluids using the free NIST chemistry web book database. *Fluid Mech Res Int* . 2017;1(1):14–18. DOI: 10.15406/fmrij.2017.01.00003

Table 3 Comparing some values of the density (in kg/m^3) at 101,325 Pa from the NIST Chemistry Web Book and two other sources

Temperature (°C)	NIST	Reference[10]	Reference[11]
10	999.7	999.7	999.8
20	998.2	998.2	998.3
30	995.6	995.7	995.7
40	992.2	992.2	992.3
50	988	988	988
60	983.2	983.2	983.1
70	977.8	977.8	977.6
80	971.8	971.8	971.6
90	965.3	965.3	965.1

Table 4 Comparing some values of the dynamic viscosity (in cP) at 101,325 Pa from the NIST Chemistry Web Book and two other sources

Temperature (°C)	NIST	Reference[10]	Reference[11]
10	1.306	1.307	1.306
20	1.002	1.002	1.002
30	0.797	0.798	0.797
40	0.653	0.653	0.653
50	0.547	0.547	0.547
60	0.466	0.466	0.466
70	0.404	0.404	0.404
80	0.354	0.354	0.354
90	0.314	0.315	0.314

Conclusion

This article gave a brief overview of the NIST Chemistry Web Book database, which can be very useful when studying, performing engineering design dealing with, or conducting research on fluids as well as other chemical species. An example was given where the constant-pressure variations of four properties were obtained using that database. A comparison between the values in this online database and other two sources for some properties of water at some conditions showed good agreement. Interested readers are encouraged to explore the capabilities of this free and user-friendly online database.

Acknowledgements

None.

Conflicts of interest

The author declares that there is no conflict of interest.

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