

DIPPR Database

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DIPPR (Design Institute for Physical Properties) (AIChE)

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DIPPR Project

1. Project 801 - Evaluated process design data.

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- Bringham Young University

Dr. Richard Rowley , Bringham Young Univ.
Dr. W. Vincent Wilding, Bringham Young Univ.
Dr. John L. Oscarson, Bringham Young Univ.

- DIPPR

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1998	1635
2000	1685
2002	1735

DIPPR 801 Project

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29 (fixed properties)

15

Fixed-value properties:

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|--|---|
| 1. Molecular weight | 16. Absolute entropy in standard state at 25° C |
| 2. Critical temperature | 17. Enthalpy of fusion at melting point |
| 3. Critical pressure | 18. Standard enthalpy of combustion at 25° C |
| 4. Critical volume | 19. Acentric Factor |
| 5. Critical compressibility factor | 20. Radius of gyration |
| 6. Melting point (at 1 atm) | 21. Solubility parameter at 25° C |
| 7. Triple point temperature | 22. Dipole moment |
| 8. Triple point pressure | 23. van der Waals volume |
| 9. Normal boiling point | 24. van der Waals area |
| 10. Liquid Molar Volume at 25° C | 25. Refractive Index |
| 11. Enthalpy of formation of ideal gas at 25° C | 26. Flash point |
| 12. Gibbs energy of formation of ideal gas at 25° C | 27. Lower flammability limit |
| 13. Absolute entropy of ideal gas at 25° C | 28. Upper flammability limit |
| 14. Enthalpy of formation in standard state at 25° C | 29. Autoignition temperature |
| 15. Gibbs energy of formation in standard state at 25° C | |

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|---|--|
| 1. Solid density (when appropriate) | 9. Second virial coefficient |
| 2. Liquid density | 10. Liquid viscosity |
| 3. Solid vapor pressure
(when appropriate) | 11. Vapor viscosity |
| 4. Vapor pressure | 12. Solid thermal conductivity
(when appropriate) |
| 5. Enthalpy of vaporization
(at saturation pressure) | 13. Liquid thermal conductivity |
| 6. Solid heat capacity
(when appropriate) | 14. Vapor thermal conductivity |
| 7. Liquid heat capacity | 15. Surface tension |
| 8. Ideal gas heat capacity | |

- Chemical identification
- Molecular formula
- Molecular structure
- Simplified Molecular Input Line Entry System (SMILES) formula
- Chemical Abstracts name
- IUPAC compound name
- Synonyms and abbreviations for the chemical name
- CAS registry number
- Chemical identification number for file

DIPPR

- (1) Standalone version
- (2) WWW Version
- (3) Educational Version

가 1685 ,
 STN International ,
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 DIADEM ,
 Brigham Young University

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Sample Chemical Database - Microsoft Internet Explorer

Address: http://dppr.byu.edu/samplesite/chemsearch.asp?Mode=Printout1&ChemID=1921

Chemical Database Property Constants

UNITS TEMPERATURE DEPENDENT PROPERTY CALCULATOR
NEW SEARCH LINKS FEEDBACK

Chemical Abstracts Name: water H₂O
 IUPAC Name: water water
 Synonyms: dihydrogen oxide ice refrigerant 718 steam
 Chemical Abstracts Number: 7732-18-5 Structural Formula: HOH

Property (click property name for references and data)	Units	Value	Note	Quality Code		
				Data type	Reliability	Source type
Molecular Weight	kg/kmol	18.0153				
Critical Temperature	K	647.13		Experimental	< 0.2%	Evaluated
Critical Pressure	Pa	2.20530E+07		Experimental	< 0.2%	Evaluated
Critical Volume	m ³ /kmol	5.59478E-02		Experimental	< 0.2%	Evaluated
Crt Compress Factor	unitless	0.229		Defined	None	Staff
Melting Point	K	273.15		Experimental	< 0.2%	Evaluated
Triple Pt. Temperature	K	273.16		Experimental	< 0.2%	Evaluated
Triple Pt. Pressure	Pa	611.73		Experimental	< 0.2%	Evaluated
Normal Boiling Point	K	373.15		Experimental	< 0.2%	Evaluated
Liq Molar Volume	m ³ /kmol	1.80691E-02		Experimental	< 0.2%	Evaluated
IG Heat of Formation	J/kmol	-2.41814E+08		Experimental	< 0.2%	Evaluated
IG Gibbs of Formation	J/kmol	-2.28390E+08	1	Defined	< 0.2%	Staff
IG Absolute Entropy	J/kmol*K	1.88724E+05		Experimental	< 0.2%	Evaluated
Std Heat of Formation	J/kmol	-2.83830E+08		Experimental	< 0.2%	Evaluated
Std Gibbs of Formation	J/kmol	-2.37174E+08	2	Defined	< 1%	Staff
Std Absolute Entropy	J/kmol*K	7.03899E+04	3	Predicted	< 1%	Staff
Heat Fusion at Melt Pt	J/kmol	6.00174E+06		Experimental	< 0.2%	Evaluated
Std Net Heat of Comb	J/kmol	0.0	4			
Acentric Factor	unitless	0.344861		Defined	None	Staff
Radius of Gyration	m	6.15000E-11		Defined	< 3%	Staff
Solubility Parameter	(J/m ³) ^{0.5}	4.78100E+04		Defined	< 3%	Staff
Dipole Moment	c*m	6.17000E-30		Experimental	< 1%	Evaluated
van der Waals Volume	m ³ /kmol	1.23700E-02	5	Defined	< 3%	Staff
van der Waals Area	m ²	2.26000E+08	6	Defined	< 5%	Staff

2. Project 805 – Experimental Data on Mixtures

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UNIFAC, ASOG

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Jurgen Gmehling – Univ. Of Oldenburg

- DDB

Stanislav Malanowski – Polish Academy of Science

Kenneth N. Marsh – University of Canturbury

W. Vincent Wilding – Bringham Young University

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Project 821 – Pure Component Liquid Vapor Pressure

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Project 851 – Critical Properties of Pure Compounds

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Project 871 – Determination of Pure component ideal gas heat of formation

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Project 911 – Environmental, Safety and Health Data Compilation

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Project 931 – Data Prediction Method

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. Project 801

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