Hydrogen

Other names:	Dihydrogen
	H2
	Molecular hydrogen
	P-HYDROGEN
	UN 1049
	UN 1966
	hydrogen (normal)
	o-Hydrogen
Inchi:	InChI=1S/H2/h1H
InchiKey:	UFHFLCQGNIYNRP-UHFFFAOYSA-N
Formula:	H2
SMILES:	[H][H]
Mol. weight [g/mol]:	2.02
CAS:	1333-74-0

Physical Properties

Property code	Value	Unit	Source
af	-0.2160		KDB
affp	422.30	kJ/mol	NIST Webbook
basg	394.70	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
gf	53.88	kJ/mol	Joback Method
gyrad	0.3710		KDB
hf	68.29	kJ/mol	Joback Method
hfus	-0.88	kJ/mol	Joback Method
hvap	15.30	kJ/mol	Joback Method
ie	15.44 ± 0.01	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.37 ± 0.05	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.44 ± 0.01	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook

ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.43 ± 0.02	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.50 ± 1.00	eV	NIST Webbook
ie	15.98	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	16.00 ± 1.00	eV	NIST Webbook
ie	15.40	eV	NIST Webbook
ie	15.43	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.43 ± 0.00	eV	NIST Webbook
ie	15.38 ± 0.00	eV	NIST Webbook
log10ws	0.18		Crippen Method
logp	0.246		Crippen Method
mcvol	10.860	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
pc	1300.00 ± 1.19	kPa	NIST Webbook
pc	1293.00	kPa	KDB
pt	7.04	kPa	KDB
pt	7.21 ± 0.04	kPa	NIST Webbook
pt	0.00	kPa	NIST Webbook
rhoc	31.04 ± 4.03	kg/m3	NIST Webbook
sgb	130.68 ± 0.00	J/mol×K	NIST Webbook
tb	20.28	K	KDB
tc	33.18 ± 0.20	K	NIST Webbook
tc	32.97	K	KDB
tf	13.81	K	KDB
tt	13.96 ± 0.05	K	NIST Webbook
tt	13.95 ± 0.06	K	NIST Webbook
tt	13.80	K	KDB
tt	0.00	K	NIST Webbook
vc	0.065	m3/kmol	KDB
zc	0.3065890		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	-10.08	J/mol×K	198.00	Joback Method
cpg	-8.36	J/mol×K	221.51	Joback Method
cpg	-6.92	J/mol×K	245.01	Joback Method
cpg	-5.74	J/mol×K	268.52	Joback Method
cpg	-4.82	J/mol×K	292.03	Joback Method
cpg	-4.12	J/mol×K	315.53	Joback Method
cpg	-3.65	J/mol×K	339.04	Joback Method
dvisc	0.0000129	Pa×s	500.00	Viscosity of H2-CO2 Mixtures at (500, 800, and 1100) K
dvisc	0.0000179	Pa×s	800.00	Viscosity of H2-CO2 Mixtures at (500, 800, and 1100) K
dvisc	0.0000226	Pa×s	1100.00	Viscosity of H2-CO2 Mixtures at (500, 800, and 1100) K
rhol	71.00	kg/m3	20.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.21426e+01
Coeff. B	-1.86390e+02
Coeff. C	4.38000e+00
Temperature range (K), min.	13.95
Temperature range (K), max.	33.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-5.20040e+00
Coeff. B	-5.25666e+01
Coeff. C	4.20040e+00
Coeff. D	-6.96717e-04
Temperature range (K), min.	14.00
Temperature range (K), max.	32.62

Datasets

Viscosity, Pa*s

Temperature, K - Gas	Pressure, kPa - Gas	Viscosity, Pa*s - Gas
294.10	34430.00	0.0000096
294.52	4680.00	0.0000090
294.52	4680.00	0.0000090
294.91	10160.00	0.0000091
295.00	81640.00	0.0000114
295.01	52730.00	0.0000102
295.02	99320.00	0.0000120
333.28	4940.00	0.0000098
333.30	48480.00	0.0000106
333.31	69110.00	0.0000112
333.31	94920.00	0.0000122
333.32	9480.00	0.0000099
400.10	28190.00	0.0000111
400.11	4830.00	0.0000111
400.11	9190.00	0.0000113
400.11	49790.00	0.0000116
400.12	71210.00	0.0000122

Reference *https://www.doi.org/10.1007/s10765-011-0999-6*

Pressure, kPa	Temperature, K	Viscosity, Pa*s
102.80	296.26	0.0000089
111.00	322.56	0.0000094
111.60	373.12	0.0000104
111.40	472.13	0.0000121
98.90	573.48	0.0000142
305.30	296.26	0.0000090
302.40	322.56	0.0000095
301.20	373.12	0.0000105
298.90	472.13	0.0000121
298.20	573.48	0.0000142
501.00	296.26	0.0000090
502.00	322.56	0.0000095
503.10	373.12	0.0000105

500.10	472.13	0.0000122
503.00	573.48	0.0000143
700.60	296.26	0.0000090
698.00	322.56	0.0000095
701.40	373.12	0.0000105
701.10	472.13	0.0000122
701.60	573.48	0.0000143

Reference *https://www.doi.org/10.1016/j.jct.2015.04.028*

Mass density, kg/m3

Temperature, K - Gas	Pressure, kPa - Gas	Mass density, kg/m3 - Gas
924.00	25112.00	6.313
914.10	24899.00	6.319
904.50	24668.00	6.324
892.30	24413.00	6.337
883.30	24272.00	6.344
874.10	24069.00	6.354
863.30	23818.00	6.366
854.70	23640.00	6.381
844.30	23469.00	6.412
834.30	23222.00	6.422
822.20	22963.00	6.441
812.90	22702.00	6.442
803.80	22451.00	6.442
792.80	22153.00	6.443
784.30	21917.00	6.444
773.40	21625.00	6.445
763.90	21370.00	6.445
753.60	21086.00	6.447
743.10	20811.00	6.447
733.60	20559.00	6.449
722.40	20262.00	6.45

Reference *https://www.doi.org/10.1021/acs.jced.9b00399*

Amount density, mol/m3

Temperature, K - Fluid (supercritical or subcritical phases)	Pressure, kPa - Fluid (supercritical or subcritical phases)	Amount density, mol/m3 - Fluid (supercritical or subcritical phases)
353.22	96078.00	21498.0
353.22	59493.00	15300.0
353.22	38699.00	10888.0
353.22	25948.00	7748.6
353.22	17741.00	5514.6
353.22	12284.00	3924.8
353.22	8580.00	2793.3
353.22	6028.00	1988.1
353.22	4251.00	1415.0
353.22	3006.00	1007.1
353.22	2129.00	716.81
353.22	1510.00	510.19
353.22	1072.00	363.13
393.22	99707.00	20498.0
393.22	62378.00	14592.0
393.22	40796.00	10388.0
393.22	27448.00	7395.6
393.22	18809.00	5265.9
393.22	13040.00	3749.8
393.22	9119.00	2670.3
393.22	6412.00	1901.7
393.22	4525.00	1354.3
393.22	3203.00	964.5
393.22	2271.00	686.9
393.22	1612.00	489.2
393.22	1145.00	348.41
353.25	99823.00	22045.0
353.25	61529.00	15689.0
353.25	39891.00	11164.0
353.25	26701.00	7944.8
353.25	18235.00	5653.8
353.25	12611.00	4023.6
353.25	8804.00	2863.5
353.25	6181.00	2037.9
353.25	4358.00	1450.3
353.25	3081.00	1032.2
353.25	2183.00	734.57

353.25	1548.00	522.79
353.25	1099.00	372.06
433.18	99763.00	19198.0
433.18	63167.00	13669.0
433.18	41617.00	9734.5
433.18	28131.00	6933.6
433.18	19337.00	4939.5
433.18	13435.00	3519.3
433.18	9409.00	2507.7
433.18	6625.00	1787.0
433.18	4682.00	1273.4
433.18	3316.00	907.49
433.18	2353.00	646.72
433.18	1673.00	460.89
433.18	1190.00	328.46
373.25	99849.00	21257.0
373.25	62030.00	15130.0
373.25	40397.00	10769.0
373.25	27113.00	7665.1
373.25	18544.00	5456.3
373.25	12844.00	3884.3
373.25	8974.00	2765.2
373.25	6306.00	1968.6
373.25	4448.00	1401.5
373.25	3146.00	997.77
373.25	2229.00	710.36
373.25	1582.00	505.73
373.25	1124.00	360.05
433.19	96737.00	18794.0
433.19	61451.00	13382.0
433.19	40570.00	9530.8
433.19	27466.00	6789.3
433.19	18887.00	4837.4
433.19	13140.00	3447.0
433.19	9208.00	2456.5
433.19	6486.00	1750.8
433.19	4585.00	1247.8
433.19	3249.00	889.41
433.19	2306.00	633.94
433.19	1640.00	451.86
433.19	1166.00	322.08
473.19	97599.00	17758.0
473.19	62556.00	12647.0
473.19	41475.00	9009.9

473.19	28177.00	6420.2
473.19	19436.00	4575.9
473.19	13542.00	3261.9
473.19	9501.00	2325.6
473.19	6699.00	1658.1
473.19	4740.00	1182.3
473.19	3362.00	843.06
473.19	2387.00	601.18
473.19	1698.00	428.7
473.19	1210.00	305.71
473.20	99349.00	17990.0
473.20	63569.00	12813.0
473.20	42153.00	9127.8
473.20	28617.00	6504.3
473.20	19728.00	4636.0
473.20	13736.00	3304.9
473.20	9636.00	2356.3
473.20	6792.00	1680.1
473.20	4805.00	1198.0
473.20	3407.00	854.3
473.20	2419.00	609.22
473.20	1722.00	434.44
473.20	1226.00	309.82

Reference *https://www.doi.org/10.1007/s10765-012-1168-2*

Thermal conductivity, W/m/K

Pressure, kPa - Fluid (supercritical or subcritical phases)	Temperature, K - Fluid (supercritical or subcritical phases)	Thermal conductivity, W/m/K - Fluid (supercritical or subcritical phases)
261.00	323.20	0.1971
261.00	323.20	0.1970
266.00	323.20	0.1971
267.00	323.20	0.1973
266.00	323.20	0.1971
5188.00	323.20	0.2031
5190.00	323.20	0.2031
5193.00	323.19	0.2032
5191.00	323.19	0.2032
5186.00	323.20	0.2029
10100.00	323.19	0.2065

10095.00	323.20	0.2065
10094.00	323.19	0.2067
10087.00	323.20	0.2067
10084.00	323.20	0.2067
19987.00	323.20	0.2147
19998.00	323.20	0.2146
20000.00	323.20	0.2142
19989.00	323.20	0.2142
19980.00	323.21	0.2147
40020.00	323.20	0.2313
40011.00	323.20	0.2304
39993.00	323.20	0.2306
39984.00	323.20	0.2311
40006.00	323.20	0.2312
59985.00	323.20	0.2488
59986.00	323.20	0.2482
59968.00	323.20	0.2483
59948.00	323.20	0.2488
59935.00	323.21	0.2488
80034.00	323.20	0.2657
80012.00	323.20	0.2648
79984.00	323.20	0.2654
79963.00	323.20	0.2659
80001.00	323.20	0.2659
97745.00	323.20	0.2813
97707.00	323.20	0.2804
97716.00	323.20	0.2820
97753.00	323.20	0.2816
97762.00	323.20	0.2814
599.00	373.23	0.2224
599.00	373.22	0.2225
598.00	373.22	0.2223
598.00	373.22	0.2224
5171.00	373.23	0.2262
5170.00	373.22	0.2262
5170.00	373.22	0.2260
5170.00	373.22	0.2261
10219.00	373.23	0.2296
10219.00	373.23	0.2295
10219.00	373.23	0.2296
10219.00	373.23	0.2298
30119.00	373.23	0.2438
30120.00	373.23	0.2437
30120.00	373.23	0.2433

30122.00	373.23	0.2432
50144.00	373.23	0.2589
50144.00	373.23	0.2588
50144.00	373.23	0.2589
70084.00	373.22	0.2757
70084.00	373.22	0.2758
70086.00	373.22	0.2758
98197.00	373.22	0.2988
98193.00	373.23	0.2983
98190.00	373.23	0.2987
98187.00	373.22	0.2983
400.00	423.27	0.2421
402.00	423.27	0.2431
403.00	423.26	0.2426
404.00	423.26	0.2418
5113.00	423.26	0.2477
5114.00	423.26	0.2476
5114.00	423.25	0.2475
10104.00	423.26	0.2499
10105.00	423.25	0.2494
10105.00	423.25	0.2502
30087.00	423.25	0.2620
30087.00	423.25	0.2619
30087.00	423.25	0.2615
50100.00	423.26	0.2771
50100.00	423.26	0.2762
50102.00	423.25	0.2764
70147.00	423.25	0.2939
70150.00	423.25	0.2927
70155.00	423.25	0.2923
96975.00	423.25	0.3140
96978.00	423.25	0.3137
96980.00	423.25	0.3142
365.00	573.28	0.2934
367.00	573.28	0.2929
369.00	573.28	0.2931
5202.00	573.27	0.3043
5202.00	573.27	0.3057
5202.00	573.27	0.3047
10155.00	573.27	0.3066
10155.00	573.27	0.3072
10156.00	573.27	0.3066
30167.00	573.27	0.3171
30167.00	573.27	0.3173

30167.00	573.27	0.3175
50208.00	573.26	0.3253
50204.00	573.27	0.3274
50202.00	573.26	0.3283
70114.00	573.27	0.3387
70106.00	573.27	0.3381
70099.00	573.27	0.3376
97001.00	573.26	0.3548
96990.00	573.26	0.3549
96979.00	573.26	0.3560
407.00	473.28	0.2609
408.00	473.29	0.2613
408.00	473.28	0.2610
409.00	473.28	0.2611
5166.00	473.28	0.2673
5167.00	473.28	0.2670
5167.00	473.28	0.2671
10065.00	473.27	0.2681
10065.00	473.27	0.2687
10065.00	473.28	0.2691
30123.00	473.27	0.2799
30124.00	473.27	0.2800
30124.00	473.27	0.2803
50176.00	473.28	0.2940
50178.00	473.28	0.2937
50179.00	473.28	0.2920
70155.00	473.27	0.3079
70156.00	473.27	0.3088
70160.00	473.27	0.3069
97460.00	473.27	0.3282
97459.00	473.27	0.3262
97457.00	473.27	0.3277
304.00	672.89	0.3296
304.00	672.89	0.3290
305.00	672.89	0.3290
306.00	672.89	0.3287
5147.00	672.88	0.3430
5143.00	672.88	0.3429
5140.00	672.88	0.3440
5137.00	672.88	0.3420
10061.00	672.88	0.3445
10060.00	672.88	0.3456
10059.00	672.88	0.3459
30074.00	672.87	0.3514

30063.00	672.87	0.3522
30056.00	672.87	0.3514
50118.00	672.87	0.3625
50107.00	672.88	0.3616
50096.00	672.87	0.3600
70044.00	672.88	0.3699
70030.00	672.88	0.3711
70012.00	672.88	0.3693
98109.00	672.87	0.3873
98074.00	672.87	0.3853
98041.00	672.87	0.3854
4315.00	373.23	0.2265
4316.00	373.23	0.2258
4316.00	373.23	0.2256
10127.00	373.23	0.2291
10126.00	373.24	0.2296
10126.00	373.23	0.2289
30053.00	373.23	0.2422
30052.00	373.23	0.2428
30052.00	373.23	0.2427
49936.00	373.23	0.2599
49936.00	373.23	0.2582
49936.00	373.23	0.2587
69998.00	373.23	0.2753
69997.00	373.23	0.2756
69998.00	373.23	0.2751
97555.00	373.23	0.3001
97558.00	373.23	0.2995
97560.00	373.23	0.2989
378.00	771.92	0.3679
381.00	771.92	0.3675
383.00	771.92	0.3671
386.00	771.92	0.3678
5144.00	771.91	0.3835
5140.00	771.92	0.3835
5136.00	771.92	0.3832
10109.00	771.91	0.3825
10100.00	771.91	0.3836
10092.00	771.91	0.3825
10086.00	771.91	0.3838
30058.00	771.91	0.3900
30036.00	771.90	0.3906
30014.00	771.91	0.3888
29994.00	771.90	0.3905

49932.00	771.90	0.3973
49904.00	771.90	0.3973
49879.00	771.91	0.3964
70520.00	771.91	0.4053
70484.00	771.90	0.4065
70444.00	771.90	0.4037
70405.00	771.90	0.4080
99205.00	771.90	0.4188
99143.00	771.90	0.4168
99008.00	771.90	0.4170
98954.00	771.90	0.4176

Reference *https://www.doi.org/10.1007/s10765-011-1052-5*

Sources

Vapor-Liquid Equilibrium for the Carbon Dioxide + Hydrogen + Methanol Ternary System:	https://www.doi.org/10.1021/je0301491
Heat capacity and thermodynamics of a synthetic two-line ferrihydrite, FeOOH·0.627H2O:	https://www.doi.org/10.1016/j.jct.2012.11.012
Standard molar enthalpies of formation in the crystalline phase of 7-hydroxy-4-methylcoumarin, 7-methoxy-4-methylcoumarin, and 6-methoxy-4-methylcoumarin:	https://www.doi.org/10.1016/j.jct.2011.04.013
Synthesis and energetics of Na, K, Rb and Cs salts by reaction with Lithium and Alkaline Earth Complex of Gadolinium with salicylic acid and 8-hydroxyquinoline:	https://www.doi.org/10.1016/j.jct.2017.07.025
Thermochemical Analysis on Rare Earth Complex of Gadolinium with salicylic acid and 8-hydroxyquinoline:	https://www.doi.org/10.1016/j.tca.2012.08.027
Solubilities of Gases in 1,1,3,3-Tetramethylguanidium Lactate at Elevated Pressures:	https://www.doi.org/10.1021/je050437s
Measuring Diffusion and Solubility of Slightly Soluble Gases in [Chmim][N-Tf2] Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00990
Solubility of Carbon Monoxide and Hydrogen in Methanol and Methyl Formate: 298-373 K and 0.3-3.5 MPa:	https://www.doi.org/10.1021/acs.jced.9b00676
Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of the 1,5- and 1,8-diaminonaphthalenes:	https://www.doi.org/10.1016/j.jct.2009.09.009
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Phase Equilibrium of Hydrogen, Carbon Dioxide, Squalene, and Squalane:	https://www.doi.org/10.1021/je800926z
Low-temperature heat capacities and standard molar enthalpy of formation of sodium benzoate C6H5COONa(s):	https://www.doi.org/10.1016/j.tca.2008.12.029
Measurement of Hydrogen Solubility in Potential Liquid Organic Hydrogen Carriers:	https://www.doi.org/10.1021/acs.jced.5b00789
Low-Temperature Heat Capacities and Standard Molar Enthalpy of Formation of Ethylenediammonium (NH3CH2CH2NH3)2[Co(CN)6]Cl2(s):	https://www.doi.org/10.1021/je901051z
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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhog:	Gas Density
rhol:	Liquid Density
rhoml:	Liquid Amount Density
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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