hydrogen fluoride

Other names: ANHYDROUS HYDROFLUORIC ACID
FLUORIC ACID
HYDROFLUORIC ACID
Inchi: InChI=1S/FH/h1H
InchiKey: KRHYYFGTRYWZRS-UHFFFAOYSA-N
Formula: FH
SMILES: F
Mol. weight [g/mol]: 20.01
CAS: 7664-39-3

Physical Properties

Property code	Value	Unit	Source
af	0.3290		KDB
affp	484.00	kJ/mol	NIST Webbook
basg	456.70	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
gf	-273.40	kJ/mol	KDB
hf	273.10	kJ/mol	KDB
hf	-273.30 ± 0.70	kJ/mol	NIST Webbook
hfus	0.52	kJ/mol	Joback Method
hvap	14.63	kJ/mol	Joback Method
ie	16.03 ± 0.01	eV	NIST Webbook
ie	16.05 ± 0.01	eV	NIST Webbook
ie	16.01 ± 0.01	eV	NIST Webbook
ie	15.92 ± 0.01	eV	NIST Webbook
ie	16.05 ± 0.01	eV	NIST Webbook
ie	16.06 ± 0.01	eV	NIST Webbook
ie	16.03 ± 0.04	eV	NIST Webbook
ie	16.06	eV	NIST Webbook
ie	15.98 ± 0.04	eV	NIST Webbook
ie	16.05	eV	NIST Webbook
ie	16.12 ± 0.04	eV	NIST Webbook
ie	16.00 ± 1.00	eV	NIST Webbook
ie	16.04	eV	NIST Webbook
ie	16.05 ± 0.04	eV	NIST Webbook
ie	16.10	eV	NIST Webbook
ie	16.04 ± 0.00	eV	NIST Webbook

ie	15.98 ± 0.04	eV	NIST Webbook
log10ws	0.14		Crippen Method
logp	0.153		Crippen Method
mcvol	12.630	ml/mol	McGowan Method
pc	6480.00	kPa	KDB
sgb	173.78 ± 0.00	J/mol×K	NIST Webbook
tb	292.70 ± 0.25	K	NIST Webbook
tb	293.00	K	KDB
tc	461.00	K	KDB
tf	189.79	K	KDB
tf	190.00 ± 0.20	K	NIST Webbook
vc	0.069	m3/kmol	KDB
zc	0.1166500		KDB
zra	0.15		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	5.03	J/mol×K	197.97	Joback Method
cpg	6.12	J/mol×K	220.47	Joback Method
cpg	7.08	J/mol×K	242.96	Joback Method
cpg	7.91	J/mol×K	265.46	Joback Method
cpg	8.63	J/mol×K	287.96	Joback Method
cpg	9.23	J/mol×K	310.46	Joback Method
cpg	9.72	J/mol×K	332.95	Joback Method
hvapt	25.20	kJ/mol	265.00	NIST Webbook
hvapt	25.20	kJ/mol	255.00	NIST Webbook
rhol	967.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66910e+01
Coeff. B	-3.86983e+03
Coeff. C	2.78700e+01
Temperature range (K), min.	189.79

Temperature range (K), max.	461.15

Datasets

Mass density, kg/m3

Temperature, K - Gas	Pressure, kPa - Gas	Mass density, kg/m3 - Gas
293.15	27.70	0.2320
293.15	29.00	0.2450
293.15	31.80	0.2820
293.15	34.50	0.3200
293.15	37.20	0.3600
293.15	41.50	0.4380
293.15	55.50	0.8020
293.15	69.30	1.311
293.15	83.30	1.954
293.15	98.60	2.86
303.15	26.40	0.2120
303.15	29.40	0.2390
303.15	34.20	0.2830
303.15	38.00	0.3200
303.15	41.50	0.3560
303.15	45.10	0.3950
303.15	52.70	0.4910
303.15	64.80	0.6940
303.15	78.00	0.9990
303.15	90.00	1.359
303.15	102.60	1.818
303.15	114.80	2.327
303.15	126.70	2.883
303.15	141.60	3.802
313.15	36.40	0.2800
313.15	39.60	0.3070
313.15	42.50	0.3310
313.15	53.30	0.4260
313.15	57.00	0.4610
313.15	62.10	0.5100
313.15	74.00	0.6440
313.15	90.70	0.8830

313.15	109.10	1.246
313.15	129.30	1.787
313.15	148.00	2.417
313.15	165.70	3.118
313.15	180.30	3.777
313.15	29.30	0.2270
313.15	35.90	0.2800
313.15	41.40	0.3260
313.15	48.30	0.3850
313.15	55.10	0.4470
313.15	68.90	0.5900
313.15	82.80	0.7670
313.15	96.60	0.9920
313.15	110.30	1.285
313.15	124.30	1.653
313.15	138.00	2.078
313.15	152.00	2.579
313.15	165.80	3.133
313.15	180.50	3.797
323.15	55.00	0.4220
323.15	100.90	0.8420
323.15	117.90	1.05
323.15	156.90	1.731
323.15	181.40	2.343
323.15	204.50	3.061
323.15	228.70	3.949
333.15	29.20	0.2180
333.15	99.90	0.7590
333.15	142.20	1.147
333.15	180.00	1.61
333.15	222.80	2.36
333.15	246.20	2.902
333.15	276.40	3.753
333.15	317.30	5.162
333.15	343.50	6.229
333.15	112.60	0.8630
333.15	163.70	1.386
333.15	199.20	1.904
333.15	234.80	2.612
333.15	270.80	3.552
333.15	305.80	4.693
333.15	341.50	6.088
343.15	24.60	0.1790
343.15	67.30	0.4880

343.15	141.70	1.05
343.15	244.70	2.094
343.15	289.60	2.791
343.15	340.60	3.856
343.15	375.40	4.777
343.15	414.80	6.034
343.15	455.30	7.553
353.15	50.50	0.3520
353.15	118.50	0.8330
353.15	189.00	1.359
353.15	279.30	2.154
353.15	334.20	2.782
353.15	391.10	3.617
353.15	450.10	4.75
353.15	509.00	6.216
353.15	583.50	8.604
363.15	78.70	0.5230
363.15	151.20	1.024
363.15	268.60	1.886
363.15	349.70	2.574
363.15	435.20	3.463
363.15	519.50	4.617
363.15	610.30	6.318
363.15	704.70	8.73
363.15	792.40	11.696
373.15	59.50	0.3890
373.15	135.10	0.8900
373.15	249.70	1.674
373.15	360.60	2.495
373.15	444.90	3.191
373.15	555.70	4.277
373.15	661.80	5.611
373.15	768.80	7.405
373.15	872.60	9.733
373.15	971.70	12.608
383.15	109.30	0.6900
383.15	256.80	1.656
383.15	388.40	2.569
383.15	518.30	3.557
383.15	666.40	4.865
383.15	794.60	6.263
383.15	928.90	8.187
383.15	1067.00	10.825
383.15	1201.00	14.245

393.15	172.30	1.108
393.15	337.70	2.178
393.15	505.50	3.335
393.15	674.90	4.611
393.15	840.70	6.052
393.15	1013.00	7.764
393.15	1175.00	10.132
393.15	1344.00	13.239
393.15	1498.00	17.048
403.15	240.60	1.492
403.15	449.30	2.829
403.15	652.20	4.216
403.15	862.30	5.791
403.15	1069.00	7.588
403.15	1278.00	9.802
403.15	1491.00	12.74
403.15	1709.00	16.83
403.15	1897.00	21.668
413.15	222.30	1.32
413.15	371.40	2.232
413.15	508.90	3.095
413.15	683.20	4.229
413.15	883.60	5.621
413.15	1059.00	6.93
413.15	1234.00	8.38
413.15	1399.00	9.914
413.15	1557.00	11.607
413.15	1728.00	13.746
413.15	2034.00	18.831
413.15	2223.00	23.108
433.15	309.80	1.785
433.15	698.60	4.1
433.15	1068.90	6.452
433.15	1452.00	9.113
433.15	1847.00	12.286
433.15	2258.00	16.303
433.15	2635.00	21.034
433.15	3001.00	27.275
433.15	3365.00	36.362
433.15	3703.00	50.976
453.15	476.50	2.703
453.15	1014.00	5.793
453.15	1550.00	9.121
453.15	2081.00	12.797

453.15	2621.00	17.077
453.15	3133.00	21.99
453.15	3651.00	28.309
453.15	4173.00	36.974
453.15	4738.00	51.158
453.15	5189.00	73.046
473.15	398.60	2.061
473.15	719.10	3.785
473.15	1113.00	5.969
473.15	1557.00	8.541
473.15	1986.00	11.159
473.15	2275.00	13.033
473.15	2590.00	15.167
473.15	2992.00	18.107
473.15	3473.00	22.184
473.15	4349.00	30.552
473.15	4995.00	38.609
473.15	5640.00	49.429
473.15	6393.00	68.899
473.15	7041.00	98.187

Reference *https://www.doi.org/10.1021/je400733m*

Sources

Distillation Separation of Hydrofluoric Acid and Nitric Acid From Acid Waste using the Salt Effect on Vapor-Liquid Equilibrium : https://www.doi.org/10.1007/s10765-010-0904-8

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7664393&Units=SI

Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers: https://www.doi.org/10.1016/j.jct.2008.09.012

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives : https://www.doi.org/10.1016/j.jct.2010.06.012

Vapor PVT and Vapor Pressure of Hydrogen Fluoride: https://www.doi.org/10.1021/je400733m

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1907

Experimental and Computational Thermochemical Study of the Three Monofluorophenol Isomers: https://www.doi.org/10.1021/je9000872

C6 Isomer of C60(CF3)12: Synthesis, properties and thermodynamic functions: https://www.doi.org/10.1016/j.jct.2013.06.004

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Experimental and computational energetic study of two halogenated 2-acetylpyrrole derivatives: https://www.doi.org/10.1016/j.jct.2010.04.001

Chemical speciation of aqueous hydrogen fluoride at various temperatures: https://www.doi.org/10.1016/j.fluid.2019.112244

Experimental thermochemical study of 2-chloroacetylpyrrole and 2-bromoacetylpyrrole at T = 298.15 K to 550.15 K: https://www.doi.org/10.1016/j.jct.2011.10.020

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: https://www.doi.org/10.1016/j.jct.2014.02.018

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Experimental and computational thermochemical study of two fluorobenzazoles: 5-fluoro-2-methylbenzoxazole and 5-fluoro-2-methylbenzothiazole: https://www.doi.org/10.1016/j.jct.2018.01.022

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhog:	Gas Density
rhol:	Liquid Density
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter