fluorine

Other names: BIFLUORIDEN
Inchi: InChI=1S/F2/c1-2
InchiKey: PXGOKWXKJXAPGV-UHFFFAOYSA-N
Formula: F2
SMILES: FF
Mol. weight [g/mol]: 38.00
CAS: 7782-41-4

Physical Properties

Property code	Value	Unit	Source
af	0.0540		KDB
affp	332.00	kJ/mol	NIST Webbook
basg	305.50	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
ea	3.17	eV	NIST Webbook
ea	2.94 ± 0.20	eV	NIST Webbook
ea	2.90 ± 0.22	eV	NIST Webbook
ea	3.08	eV	NIST Webbook
ea	2.80 ± 0.30	eV	NIST Webbook
ea	3.00	eV	NIST Webbook
ea	3.08 ± 0.10	eV	NIST Webbook
ea	3.00 ± 0.07	eV	NIST Webbook
ea	3.12 ± 0.07	eV	NIST Webbook
gf	-440.50	kJ/mol	Joback Method
hf	-435.55	kJ/mol	Joback Method
hfus	1.92	kJ/mol	Joback Method
hvap	13.96	kJ/mol	Joback Method
ie	15.70	eV	NIST Webbook
ie	15.74	eV	NIST Webbook
ie	15.69 ± 0.01	eV	NIST Webbook
ie	15.70	eV	NIST Webbook
ie	15.69 ± 0.01	eV	NIST Webbook
ie	15.70	eV	NIST Webbook
ie	15.70	eV	NIST Webbook
ie	15.70 ± 0.00	eV	NIST Webbook
ie	15.70	eV	NIST Webbook
ie	15.69	eV	NIST Webbook

ie	15.70 ± 0.02	eV	NIST Webbook
ie	15.70 ± 0.01	eV	NIST Webbook
ie	15.70 ± 0.00	eV	NIST Webbook
log10ws	-0.52		Crippen Method
logp	0.840		Crippen Method
mcvol	14.400	ml/mol	McGowan Method
nfpah	%!d(float64=4)		KDB
nfpas	%!d(float64=3)		KDB
pc	5172.00	kPa	KDB
sgb	202.79 ± 0.01	J/mol×K	NIST Webbook
tb	85.03	K	KDB
tb	85.20 ± 0.30	K	NIST Webbook
tc	144.13	K	KDB
tc	144.00 ± 1.00	K	NIST Webbook
tf	55.20 ± 0.30	K	NIST Webbook
tf	53.49	K	KDB
vc	0.066	m3/kmol	KDB
zc	0.2848470		KDB
zra	0.29		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	22.60	J/mol×K	305.67	Joback Method
cpg	20.14	J/mol×K	197.94	Joback Method
cpg	20.65	J/mol×K	219.49	Joback Method
cpg	21.15	J/mol×K	241.03	Joback Method
cpg	21.64	J/mol×K	262.58	Joback Method
cpg	22.13	J/mol×K	284.12	Joback Method
cpg	23.07	J/mol×K	327.21	Joback Method
rhol	1510.00	kg/m3	85.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38604e+01

Coeff. B	-7.37058e+02
Coeff. C	-5.20000e+00
Temperature range (K), min.	53.48
Temperature range (K), max.	144.31

Sources

Isomorphism and phase diagram of Pb5(PO4)3F-Pb5(PO4)3Cl system:	https://www.doi.org/10.1016/j.tca.2010.11.020
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard molar enthalpies of formation of copper(II) beta-diketonates and monomethio beta-diketonates:	https://www.doi.org/10.1016/j.jct.2005.08.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1951
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7782414&Units=SI
Experimental and computational thermochemical study of two fluorobenzazoles:	https://www.doi.org/10.1016/j.jct.2018.01.022
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
5-fluoro-2-methylbenzoxazole and 5-fluoro-2-methylbenzothiazole:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
ea:	Electron affinity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure

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