3H-Diazirine, 3,3-difluoro-

Other names: Difluoro-3H-diazirine
Inchi: InChI=1S/CF2N2/c2-1(3)4-5-1
InchiKey: FADBWTVPDJZQOE-UHFFFAOYSA-N
Formula: CF2N2
SMILES: FC1(F)N=N1
Mol. weight [g/mol]: 78.02
CAS: 693-85-6

Physical Properties

Property code	Value	Unit	Source
gf	-113.30	kJ/mol	Joback Method
hf	-168.43	kJ/mol	Joback Method
hfus	7.84	kJ/mol	Joback Method
hvap	27.66	kJ/mol	Joback Method
ie	11.20	eV	NIST Webbook
log10ws	-0.70		Crippen Method
logp	1.002		Crippen Method
mcvol	33.290	ml/mol	McGowan Method
pc	7049.79	kPa	Joback Method
tb	334.36	K	Joback Method
tc	535.84	K	Joback Method
tf	287.89	K	Joback Method
vc	0.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	66.08	J/mol×K	334.36	Joback Method
cpg	73.65	J/mol×K	367.94	Joback Method
cpg	80.48	J/mol×K	401.52	Joback Method
cpg	86.62	J/mol×K	435.10	Joback Method
cpg	92.15	J/mol×K	468.68	Joback Method
cpg	97.12	J/mol×K	502.26	Joback Method
cpg	101.62	J/mol×K	535.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693856&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume