N,N,1,1-Tetrafluoro-1-chloromethylamine

Other names: Difluoro(difluorochloromethyl)amine
Inchi: InChI=1S/CClF4N/c2-1(3,4)7(5)6
InchiKey: NLMHABPAWPTMMR-UHFFFAOYSA-N
Formula: CClF4N
SMILES: FN(F)C(F)(F)Cl
Mol. weight [g/mol]: 137.46
CAS: 13880-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-720.01	kJ/mol	Joback Method
hf	-805.37	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	19.68	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.847		Crippen Method
mcvol	54.250	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	266.00	K	Joback Method
tc	406.98	K	Joback Method
tf	168.20	K	Joback Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.42	J/mol×K	266.00	Joback Method
cpg	90.42	J/mol×K	289.50	Joback Method
cpg	95.10	J/mol×K	312.99	Joback Method
cpg	99.49	J/mol×K	336.49	Joback Method
cpg	103.60	J/mol×K	359.99	Joback Method
cpg	107.43	J/mol×K	383.49	Joback Method
cpg	110.99	J/mol×K	406.98	Joback Method
hvapt	26.60	kJ/mol	243.00	NIST Webbook

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=C13880712&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
hvapt:	Enthalpy of vaporization at a given temperature
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