Ditrifluoromethyl(chlorocarbonyloxy)amine

Other names: O-(chloroformyl)-N,N-bis(trifluoromethyl)hydroxylamine
Inchi: InChI=1S/C3ClF6NO2/c4-1(12)13-11(2(5,6)7)3(8,9)10
InchiKey: ADPIJPFGLVDJEK-UHFFFAOYSA-N
Formula: C3ClF6NO2
SMILES: O=C(Cl)ON(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 231.48
CAS: 15496-01-2

Physical Properties

Property code	Value	Unit	Source
gf	-1323.87	kJ/mol	Joback Method
hf	-1492.42	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	30.36	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.618		Crippen Method
mcvol	93.410	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	383.36	K	Joback Method
tc	536.76	K	Joback Method
tf	266.50	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.30	J/mol×K	511.19	Joback Method
cpg	196.73	J/mol×K	383.36	Joback Method
cpg	203.75	J/mol×K	408.93	Joback Method
cpg	210.29	J/mol×K	434.49	Joback Method
cpg	216.39	J/mol×K	460.06	Joback Method
cpg	222.05	J/mol×K	485.63	Joback Method
cpg	232.16	J/mol×K	536.76	Joback Method
hvapt	34.50	kJ/mol	256.50	NIST Webbook

Sources

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=C15496012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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