

Ethanamine, N-chloro-N,1,1-trifluoro-

Other names:	Ethylamine, N-chloro-N,1,1-trifluoro-N-chloro-N,1,1-trifluoroethanamine
Inchi:	InChI=1S/C2H3ClF3N/c1-2(4,5)7(3)6/h1H3
InchiKey:	ITYSTFRAOPTVON-UHFFFAOYSA-N
Formula:	C2H3ClF3N
SMILES:	CC(F)(F)N(F)Cl
Mol. weight [g/mol]:	133.50
CAS:	16276-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-516.78	kJ/mol	Joback Method
hf	-629.90	kJ/mol	Joback Method
hfus	9.98	kJ/mol	Joback Method
hvap	22.73	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.939		Crippen Method
mvol	66.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	289.61	K	Joback Method
tc	441.48	K	Joback Method
tf	178.88	K	Joback Method
vc	0.258	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.51	J/molxK	289.61	Joback Method
cpg	111.11	J/molxK	314.92	Joback Method
cpg	117.33	J/molxK	340.23	Joback Method
cpg	123.18	J/molxK	365.54	Joback Method
cpg	128.67	J/molxK	390.85	Joback Method
cpg	133.82	J/molxK	416.16	Joback Method
cpg	138.65	J/molxK	441.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16276452&Units=SI
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

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

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