

Ethanamine, 2-chloro-N,N-dimethyl-

Other names:	(2-Chloroethyl)dimethylamine Ethylamine, 2-chloro-N,N-dimethyl- Chloro(dimethylamino)ethane «beta»-Chloroethyldimethylamine N-(2-Chloroethyl)dimethylamine Dimethylaminoethyl chloride «beta»-(Dimethylamino)ethyl chloride 2-Dimethylaminoethylchloride Dimethyl(2-chloroethyl)amine HN 1 Nitrogen half mustard 1-Dimethylamino-2-chloroethane N,N-Dimethyl-2-chloroethylamine
Inchi:	InChI=1S/C4H10ClN/c1-6(2)4-3-5/h3-4H2,1-2H3
InchiKey:	WQMAANNAZKNUDL-UHFFFAOYSA-N
Formula:	C4H10ClN
SMILES:	CN(C)CCCl
Mol. weight [g/mol]:	107.58
CAS:	107-99-3

Physical Properties

Property code	Value	Unit	Source
gf	81.65	kJ/mol	Joback Method
hf	-74.10	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	30.93	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.787		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	746.00		NIST Webbook
rinpol	750.38		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	750.38		NIST Webbook
tb	340.79	K	Joback Method
tc	512.15	K	Joback Method
tf	197.23	K	Joback Method

vc	0.327	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.13	J/mol×K	340.79	Joback Method
cpg	151.09	J/mol×K	369.35	Joback Method
cpg	159.67	J/mol×K	397.91	Joback Method
cpg	167.87	J/mol×K	426.47	Joback Method
cpg	175.72	J/mol×K	455.03	Joback Method
cpg	183.22	J/mol×K	483.59	Joback Method
cpg	190.38	J/mol×K	512.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107993&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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