Ethanamine, 2-chloro-N,N-diethyl-

Other names:	Triethylamine, 2-chloro- N-(2-Chloroethyl)diethylamine (2-Chloroethyl)diethylamine «beta»-Chlorotriethylamine 2-Chlorotriethylamine 2-(Diethylamino)chloroethane Diethylaminoethyl chloride «beta»-(Diethylamino)ethyl chloride N-Diethylaminoethyl chloride 2-(Diethylamino)ethyl chloride Diethyl(2-chloroethyl)amine 1-Chloro-2-(diethylamino)ethane 1-Diethylamino-2-chloroethane N,N-Diethyl-2-chloroethylamine
Inchi:	InChI=1S/C6H14ClN/c1-3-8(4-2)6-5-7/h3-6H2,1-2H3
InchiKey:	YMDNODNLFSHHCV-UHFFFAOYSA-N
Formula:	C6H14ClN
SMILES:	CCN(CC)CCCl
Mol. weight [g/mol]:	135.63
CAS:	100-35-6

Physical Properties

Property code	Value	Unit	Source
gf	98.49	kJ/mol	Joback Method
hf	-115.38	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.567		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	911.29		NIST Webbook
rinpol	911.29		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	901.00		NIST Webbook
tb	386.55	K	Joback Method
tc	557.47	K	Joback Method

tf	219.77	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.04	J/mol×K	386.55	Joback Method
cpg	224.63	J/mol×K	415.04	Joback Method
cpg	235.73	J/mol×K	443.52	Joback Method
cpg	246.35	J/mol×K	472.01	Joback Method
cpg	256.50	J/mol×K	500.50	Joback Method
cpg	266.21	J/mol×K	528.99	Joback Method
cpg	275.49	J/mol×K	557.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100356&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
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