N-Methyl-N-propyl aminoethyl-2-chloride

Other names: ethanamine, 2-chloro, N-methyl, N-propyl
Inchi: InChI=1S/C6H14ClN/c1-3-5-8(2)6-4-7/h3-6H2,1-2H3
InchiKey: HOOCCUKDJXWUCS-UHFFFAOYSA-N
Formula: C6H14ClN
SMILES: CCCN(C)CCCl
Mol. weight [g/mol]: 135.63

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	923.16		NIST Webbook
rinpol	923.16		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360311&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