N-Isopropyl-N-methyl aminoethyl-2-chloride

Other names: ethanamine, 2-chloro, N-methyl, N-isopropyl
Inchi: InChI=1S/C6H14ClN/c1-6(2)8(3)5-4-7/h6H,4-5H2,1-3H3
InchiKey: LXARWMYOCCWJQI-UHFFFAOYSA-N
Formula: C6H14ClN
SMILES: CC(C)N(C)CCCl
Mol. weight [g/mol]: 135.63

Physical Properties

Property code	Value	Unit	Source
gf	96.05	kJ/mol	Joback Method
hf	-120.66	kJ/mol	Joback Method
hfus	14.99	kJ/mol	Joback Method
hvap	34.99	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.565		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	922.59		NIST Webbook
rinpol	922.59		NIST Webbook
tb	386.11	K	Joback Method
tc	561.03	K	Joback Method
tf	204.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.96	J/mol×K	386.11	Joback Method
cpg	224.91	J/mol×K	415.26	Joback Method
cpg	236.34	J/mol×K	444.42	Joback Method
cpg	247.26	J/mol×K	473.57	Joback Method
cpg	257.70	J/mol×K	502.73	Joback Method
cpg	267.66	J/mol×K	531.88	Joback Method
cpg	277.16	J/mol×K	561.03	Joback Method

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=U360310&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
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