N-Isopropyl-N-propyl aminoethyl-2-chloride

Other names: ethanamine, 2-chloro, N-propyl, N-isopropyl
Inchi: InChI=1S/C8H18ClN/c1-4-6-10(7-5-9)8(2)3/h8H,4-7H2,1-3H3
InchiKey: WUYUGBPLXZIKGW-UHFFFAOYSA-N
Formula: C8H18ClN
SMILES: CCCN(CCCl)C(C)C
Mol. weight [g/mol]: 163.69

Physical Properties

Property code	Value	Unit	Source
gf	112.89	kJ/mol	Joback Method
hf	-161.94	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.346		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1065.40		NIST Webbook
rinpol	1065.40		NIST Webbook
tb	431.87	K	Joback Method
tc	604.95	K	Joback Method
tf	227.31	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.35	J/mol×K	431.87	Joback Method
cpg	307.46	J/mol×K	460.72	Joback Method
cpg	320.96	J/mol×K	489.56	Joback Method
cpg	333.87	J/mol×K	518.41	Joback Method
cpg	346.21	J/mol×K	547.26	Joback Method
cpg	357.98	J/mol×K	576.10	Joback Method
cpg	369.22	J/mol×K	604.95	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=U360316&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