N,N-Dipropyl aminoethyl-2-chloride

Other names: ethanamine, 2-chloro, N,N-dipropyl
Inchi: InChI=1S/C8H18ClN/c1-3-6-10(7-4-2)8-5-9/h3-8H2,1-2H3
InchiKey: QKWHKHPUGFKVCP-UHFFFAOYSA-N
Formula: C8H18ClN
SMILES: CCCN(CCC)CCCl
Mol. weight [g/mol]: 163.69

Physical Properties

Property code	Value	Unit	Source
gf	115.33	kJ/mol	Joback Method
hf	-156.66	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	39.83	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	2.347		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1079.24		NIST Webbook
rinpol	1079.24		NIST Webbook
tb	432.31	K	Joback Method
tc	601.66	K	Joback Method
tf	242.31	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.33	J/mol×K	432.31	Joback Method
cpg	307.06	J/mol×K	460.54	Joback Method
cpg	320.21	J/mol×K	488.76	Joback Method
cpg	332.80	J/mol×K	516.99	Joback Method
cpg	344.84	J/mol×K	545.21	Joback Method
cpg	356.35	J/mol×K	573.44	Joback Method
cpg	367.36	J/mol×K	601.66	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=U360315&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