2-Propanamine, N-(2-chloroethyl)-N-(1-methylethyl)-

Other names: «beta»-Diisopropylaminoethyl chloride
Diisopropylaminoethyl chloride
N-(2-Chloroethyl)diisopropylamine
N,N-Diisopropyl-2-chloroethylamine
Triethylamine, 2-chloro-1',1''-dimethyl-
1-(Diisopropylamino)-2-chloroethane
1-Chloro-2-diisopropylaminoethane
2-(Diisopropylamino)ethyl chloride
2-Chloro-N,N-diisopropylethanamine
2-Chloro-N,N-diisopropylethylamine
Diisopropylamine, N-(2-chloroethyl)-
Diisopropyl-(2-chloro-ethyl)-amine
NSC 11785

Inchi: InChI=1S/C8H18ClN/c1-7(2)10(6-5-9)8(3)4/h7-8H,5-6H2,1-4H3

InchiKey: DBVADBHSJCWFKI-UHFFFAOYSA-N

Formula: C8H18ClN

SMILES: CC(C)N(CCCl)C(C)C

Mol. weight [g/mol]: 163.69

CAS: 96-79-7

Physical Properties

Property code	Value	Unit	Source
gf	110.45	kJ/mol	Joback Method
hf	-167.22	kJ/mol	Joback Method
hfus	16.65	kJ/mol	Joback Method
hvap	39.05	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.344		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1049.05		NIST Webbook
tb	431.43	K	Joback Method
tc	608.37	K	Joback Method
tf	212.31	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.36	J/mol×K	431.43	Joback Method
cpg	307.88	J/mol×K	460.92	Joback Method
cpg	321.74	J/mol×K	490.41	Joback Method
cpg	334.98	J/mol×K	519.90	Joback Method
cpg	347.62	J/mol×K	549.39	Joback Method
cpg	359.66	J/mol×K	578.88	Joback Method
cpg	371.14	J/mol×K	608.37	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=C96797&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