BIS(2-CHLOROETHYL)AMINE

Other names:	N,N-Bis-(«beta»-chloroethyl)-amine
	Bis-«beta»-chloroethylamine
	NH-lost
	Nor-nitrogen mustard
	NSC-10873
	Ethanamine, 2-chloro-N-(2-chloroethyl)-
	2,2'-Dichlorodiethylamine
	Bis(beta-chloroethyl)amine
	Bis(2-chloroethyl)amine
	Bis(chloroethyl)amine
	Di(2-chloroethyl)amine
	N,N-Bis(2-chloroethane)amine
	Nor-HN2
	Nor-mechlorethamine
	Nor-mustard
	N,N-Bis(2-chloroethyl)amine
	Nor-N-mustard
	Nitrogen mustard
Inchi:	InChI=1S/C4H9Cl2N/c5-1-3-7-4-2-6/h7H,1-4H2
InchiKey:	TXFLGZOGNOOEFZ-UHFFFAOYSA-N
Formula:	C4H9Cl2N
SMILES:	ClCCNCCCl
Mol. weight [g/mol]:	142.03

Physical Properties

Property code	Value	Unit	Source
hfus	19.61	kJ/mol	Joback Method
logp	1.054		Crippen Method
mcvol	101.680	ml/mol	McGowan Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.49	J/mol×K	415.95	Joback Method
cpg	184.77	J/mol×K	447.13	Joback Method
cpg	192.66	J/mol×K	478.30	Joback Method
cpg	200.19	J/mol×K	509.48	Joback Method
cpg	207.35	J/mol×K	540.66	Joback Method
cpg	214.18	J/mol×K	571.84	Joback Method
cpg	220.66	J/mol×K	603.01	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C334225&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices