Bis(2-chloroethyl)methylamine

Other names:

2,2'-Dichloro-N-methyldiethylamine
2,2'-Dichlorodiethyl-methylamine
2-Chloro-N-(2-chloroethyl)-N-methylethanamine
55-86-7 (chloride)
Bis(b-chloroethyl)methylamine
Bis(«beta»-chloroethyl)methylamine
Bis(Â«betaÂ»-chloroethyl)methylamine
Chlorethazine
Chlormethine
Cloramin
Di(2-chloroethyl)methylamine
Dichlor amine
Diethylamine, 2,2'-dichloro-N-methyl-
ENT-25294
Ethanamine, 2-chloro-N-(2-chloroethyl)-N-methyl-
HN2
HN2 (amine)
MBA
Mechlorethamine
Mechloroethamine
Mecloretamina
Methylbis(2-chloroethyl)amine
Methylbis(«beta»-chloroethyl)amine
Methylbis(Â«betaÂ»-chloroethyl)amine
Methyldi(2-chloroethyl)amine
Mustargen
Mustine
Mustine Note
N,N-Bis(2-chloroethyl)methylamine
N,N-Di(chloroethyl)methylamine
N-Methyl-2,2'-dichlorodiethylamine
N-Methyl-bis(2-chloroethyl)amine
N-Methyl-bis(«beta»-chloroethyl)amine
N-Methyl-bis(Â«betaÂ»-chloroethyl)amine
N-Methyl-bis-chloraethylamin
N-Methyl-lost
NSC 762
Nitrogen mustard
T-1024
TL 146

	«beta»,«beta»'-Dichlorodiethyl-N-methylamine
	Â«betaÂ»,Â«betaÂ»'-Dichlorodiethyl-N-methylamine
Inchi:	InChI=1S/C5H11Cl2N/c1-8(4-2-6)5-3-7/h2-5H2,1H3
InchiKey:	HAWPXGHAZFHHAD-UHFFFAOYSA-N
Formula:	C5H11Cl2N
SMILES:	CN(CCCl)CCCl
Mol. weight [g/mol]:	156.05
CAS:	51-75-2

Physical Properties

Property code	Value	Unit	Source
gf	78.14	kJ/mol	Joback Method
hf	-110.48	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	37.54	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	1.396		Crippen Method
mcvol	115.770	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1083.26		NIST Webbook
rinpol	1084.87		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1566.30		NIST Webbook
ripol	1574.00		NIST Webbook
tb	401.10	K	Joback Method
tc	580.59	K	Joback Method
tf	238.42	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.72	J/mol×K	401.10	Joback Method
cpg	212.77	J/mol×K	431.01	Joback Method
cpg	222.35	J/mol×K	460.93	Joback Method
cpg	231.46	J/mol×K	490.84	Joback Method
cpg	240.12	J/mol×K	520.76	Joback Method
cpg	248.36	J/mol×K	550.67	Joback Method
cpg	256.18	J/mol×K	580.59	Joback Method
hvapt	54.60	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35150e+01
Coeff. B	-4.71471e+03
Temperature range (K), min.	356.43
Temperature range (K), max.	574.72

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=C51752&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume