p-N,N-Bis(2-chloroethyl)aminobenzoic acid

Other names:	Benzoic acid nitrogen mustard
	Benzoic acid, p-(bis(2-chloroethyl)amino)-
	Benzoic acid, 4-(bis(2-chloroethyl)amino)-
	4-(Bis(2-chloroethyl)amino)benzoic acid
Inchi:	InChI=1S/C11H13Cl2NO2/c12-5-7-14(8-6-13)10-3-1-9(2-4-10)11(15)16/h1-4H,5-8H2,(H,
InchiKey:	PCLQMXVMRDPVKX-UHFFFAOYSA-N
Formula:	C11H13Cl2NO2
SMILES:	O=C(O)c1ccc(N(CCCl)CCCl)cc1
Mol. weight [g/mol]:	262.13
CAS:	1141-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.30	kJ/mol	Joback Method
hf	-274.07	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.669		Crippen Method
mcvol	183.990	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	716.09	K	Joback Method
tc	919.73	K	Joback Method
tf	455.73	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.58	J/mol×K	716.09	Joback Method
cpg	469.98	J/mol×K	750.03	Joback Method
cpg	479.68	J/mol×K	783.97	Joback Method
cpg	488.71	J/mol×K	817.91	Joback Method
cpg	497.11	J/mol×K	851.85	Joback Method

cpg	504.93	J/mol×K	885.79	Joback Method
cpg	512.22	J/mol×K	919.73	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1141373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume