Chloramben methyl

Other names:	2,5-Dichloro-3-aminobenzoic acid, methyl ester
	3-Amino-2,5-dichlorobenzoic acid, methyl ester
	Amchem 65-81-b
	Amiben, methyl ester
	Benzoic acid, 3-amino-2,5-dichloro-, methylated
	Chloramben, methyl ester
	Methyl 3-amino-2,5-dichlorobenzoate
	Methyl chloramben
	NSC 190368
Inchi:	InChI=1S/C8H7Cl2NO2/c1-13-8(12)5-2-4(9)3-6(11)7(5)10/h2-3H,11H2,1H3
InchiKey:	DTSSCQVCVYZGSI-UHFFFAOYSA-N
Formula:	C8H7Cl2NO2
SMILES:	COC(=O)c1cc(Cl)cc(N)c1Cl
Mol. weight [g/mol]:	220.06

Physical Properties

Property code	Value	Unit	Source
hf	-327.02	kJ/mol	Cheméo Relay (1.0)
hfus	25.73	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-3.26		Aqueous Solubility Prediction Method
logp	2.362		Crippen Method
mcvol	141.720	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	574.51	K	Cheméo Relay (1.0)
tf	335.09 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.36	J/mol×K	647.74	Joback Method
cpg	314.51	J/mol×K	687.68	Joback Method

cpg	323.02	J/mol×K	727.62	Joback Method
cpg	330.92	J/mol×K	767.55	Joback Method
cpg	338.18	J/mol×K	807.49	Joback Method
cpg	344.83	J/mol×K	847.43	Joback Method
cpg	350.84	J/mol×K	887.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7286842&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point