Benzoic acid, 3-amino-2,5-dichloro-, methyl ester

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
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]: 220.05

CAS: 7286-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-91.33	kJ/mol	Joback Method
hf	-248.82	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
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	647.74	K	Joback Method
tc	887.37	K	Joback Method
tf	335.09 ± 0.50	K	NIST Webbook
vc	0.526	m3/kmol	Joback Method

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

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

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