3-Amino-2,5-dichlorobenzoic acid, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C11H12Cl2N2O2/c1-15(2)6-14-9-5-7(12)4-8(10(9)13)11(16)17-3/h4-6H,1-3H3

InchiKey: HYZFQWSMJIFMQX-UHFFFAOYSA-N

Formula: C11H12Cl2N2O2

SMILES: COC(=O)c1cc(Cl)cc(N=CN(C)C)c1Cl

Mol. weight [g/mol]: 275.13

Physical Properties

Property code	Value	Unit	Source
hf	-194.78	kJ/mol	Joback Method
hvap	67.62	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.001		Crippen Method
mcvol	189.670	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	732.97	K	Joback Method
tc	962.73	K	Joback Method

Sources

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

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=U375839&Units=SI

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature