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

Inchi: InChI=1S/C12H14Cl2N2O2/c1-4-18-12(17)9-5-8(13)6-10(11(9)14)15-7-16(2)3/h5-7H,4H2

InchiKey: FEAXMWOCNZRBLT-UHFFFAOYSA-N

Formula: C12H14Cl2N2O2

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

Mol. weight [g/mol]: 289.16

Physical Properties

Property code	Value	Unit	Source
hf	-215.42	kJ/mol	Joback Method
hvap	69.85	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.391		Crippen Method
mcvol	203.760	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2259.00		NIST Webbook
tb	755.85	K	Joback Method
tc	981.76	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=U375838&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