3-Amino-2,3-dihydrobenzoic acid, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C11H16N2O2/c1-13(2)8-12-10-6-4-5-9(7-10)11(14)15-3/h4-6,8,10H,7H2,1-3H3

InchiKey: MRZXRVKVGAEXPV-UHFFFAOYSA-N

Formula: C11H16N2O2

SMILES: COC(=O)C1=CC=CC(N=CN(C)C)C1

Mol. weight [g/mol]: 208.26

Physical Properties

Property code	Value	Unit	Source
hf	-207.01	kJ/mol	Joback Method
hvap	56.27	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.004		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	639.34	K	Joback Method
tc	858.81	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=U375820&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