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

Inchi: InChI=1S/C12H18N2O2/c1-4-16-12(15)10-6-5-7-11(8-10)13-9-14(2)3/h5-7,9,11H,4,8H2,

InchiKey: OJHMIGMZFSGXTR-UHFFFAOYSA-N

Formula: C12H18N2O2

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

Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
hf	-227.65	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.394		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	662.22	K	Joback Method
tc	877.98	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375819&Units=SI

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

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