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

Inchi: InChI=1S/C14H22N2O2/c1-4-5-9-18-14(17)12-7-6-8-13(10-12)15-11-16(2)3/h6-8,11,13H

InchiKey: NRMQOXMKLOAYIF-UHFFFAOYSA-N

Formula: C14H22N2O2

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

Mol. weight [g/mol]: 250.34

Physical Properties

Property code	Value	Unit	Source
hf	-268.93	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.174		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	707.98	K	Joback Method
tc	917.39	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375818&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