DL-3-Aminoisobutyric acid, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C11H22N2O2/c1-5-6-7-15-11(14)10(2)8-12-9-13(3)4/h9-10H,5-8H2,1-4H3

InchiKey: ITSLBBQPCZTJEH-UHFFFAOYSA-N

Formula: C11H22N2O2

SMILES: CCCCOC(=O)C(C)CN=CN(C)C

Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
hf	-370.70	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.556		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
tb	616.05	K	Joback Method
tc	803.58	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=U375501&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