DL-«beta»-Homoleucine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C11H22N2O2/c1-9(2)6-10(7-11(14)15-5)12-8-13(3)4/h8-10H,6-7H2,1-5H3

InchiKey: SMJAOOKXGQQXII-UHFFFAOYSA-N

Formula: C11H22N2O2

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

Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
hf	-375.98	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.554		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
tb	615.61	K	Joback Method
tc	806.50	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375790&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