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

Inchi: InChI=1S/C14H20N2O2/c1-16(2)11-15-13(10-14(17)18-3)9-12-7-5-4-6-8-12/h4-8,11,13H

InchiKey: XEXIYJWBCDYJSK-UHFFFAOYSA-N

Formula: C14H20N2O2

SMILES: COC(=O)CC(Cc1ccccc1)N=CN(C)C

Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
hf	-196.09	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.751		Crippen Method
mcvol	207.460	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	711.37	K	Joback Method
tc	926.09	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375787&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

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

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