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

Inchi: InChI=1S/C15H22N2O2/c1-4-19-15(18)11-14(16-12-17(2)3)10-13-8-6-5-7-9-13/h5-9,12,1

InchiKey: CYHYOLROWOYBID-UHFFFAOYSA-N

Formula: C15H22N2O2

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

Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
hf	-216.73	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.141		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	1848.00		NIST Webbook
tb	734.25	K	Joback Method
tc	946.05	K	Joback Method

Sources

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=U375786&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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