DL-Phenylalanine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C13H18N2O2/c1-15(2)10-14-12(13(16)17-3)9-11-7-5-4-6-8-11/h4-8,10,12H,9H

InchiKey: LERRDKPNOROUQK-UHFFFAOYSA-N

Formula: C13H18N2O2

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

Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
hf	-175.45	kJ/mol	Joback Method
hvap	60.93	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.361		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	688.49	K	Joback Method
tc	906.57	K	Joback Method

Sources

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=U375701&Units=SI

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

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