DL-Phenylalanine, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C16H24N2O2/c1-4-5-11-20-16(19)15(17-13-18(2)3)12-14-9-7-6-8-10-14/h6-10

InchiKey: NYEHPAUBKFWVRE-UHFFFAOYSA-N

Formula: C16H24N2O2

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

Mol. weight [g/mol]: 276.37

Physical Properties

Property code	Value	Unit	Source
hf	-237.37	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.531		Crippen Method
mcvol	235.640	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	757.13	K	Joback Method
tc	966.48	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=U375699&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