p-Fluoro-L-phenylalanine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C13H17FN2O2/c1-16(2)9-15-12(13(17)18-3)8-10-4-6-11(14)7-5-10/h4-7,9,12H

InchiKey: CGXMYDPHKSASGO-UHFFFAOYSA-N

Formula: C13H17FN2O2

SMILES: COC(=O)C(Cc1ccc(F)cc1)N=CN(C)C

Mol. weight [g/mol]: 252.28

Physical Properties

Property code	Value	Unit	Source
hf	-383.03	kJ/mol	Joback Method
hvap	60.78	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.500		Crippen Method
mcvol	195.140	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	692.74	K	Joback Method
tc	902.72	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=U375828&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