D-p-Chlorophenylalanine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C13H17ClN2O2/c1-16(2)9-15-12(13(17)18-3)8-10-4-6-11(14)7-5-10/h4-7,9,12H

InchiKey: PCXLDSNKICKJPT-UHFFFAOYSA-N

Formula: C13H17ClN2O2

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

Mol. weight [g/mol]: 268.74

Physical Properties

Property code	Value	Unit	Source
hf	-202.66	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.014		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	730.90	K	Joback Method
tc	952.78	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=U375824&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