3-Amino-3-(4-methylphenyl)propionic acid, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C14H20N2O2/c1-11-5-7-12(8-6-11)13(9-14(17)18-4)15-10-16(2)3/h5-8,10,13H

InchiKey: YTGWOQVCFBROLR-UHFFFAOYSA-N

Formula: C14H20N2O2

SMILES: COC(=O)CC(N=CN(C)C)c1ccc(C)cc1

Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
hf	-207.56	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.189		Crippen Method
mcvol	207.460	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	716.35	K	Joback Method
tc	931.88	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375837&Units=SI

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

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