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

Inchi: InChI=1S/C15H22N2O2/c1-5-19-15(18)10-14(16-11-17(3)4)13-8-6-12(2)7-9-13/h6-9,11,1

InchiKey: FTIJNKHTSYBGPS-UHFFFAOYSA-N

Formula: C15H22N2O2

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

Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
hf	-228.20	kJ/mol	Joback Method
hvap	66.05	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.579		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1912.00		NIST Webbook
tb	739.23	K	Joback Method
tc	951.82	K	Joback Method

Sources

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=U375836&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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