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

Inchi: InChI=1S/C14H19FN2O2/c1-4-19-14(18)9-13(16-10-17(2)3)11-5-7-12(15)8-6-11/h5-8,10

InchiKey: YWMNYZKYHQYREJ-UHFFFAOYSA-N

Formula: C14H19FN2O2

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

Mol. weight [g/mol]: 266.31

Physical Properties

Property code	Value	Unit	Source
hf	-403.67	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.410		Crippen Method
mcvol	209.230	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1805.00		NIST Webbook
tb	715.62	K	Joback Method
tc	922.86	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=U375834&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