

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

Inchi:	InChI=1S/C13H17FN2O2/c1-16(2)9-15-12(8-13(17)18-3)10-4-6-11(14)7-5-10/h4-7,9,12H
InchiKey:	FFMCISCRMFDWSV-UHFFFAOYSA-N
Formula:	C13H17FN2O2
SMILES:	COC(=O)CC(N=CN(C)C)c1ccc(F)cc1
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	-2.25		Crippen Method
logp	2.020		Crippen Method
mcvol	195.140	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		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=U375835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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