DL-2-fluorophenylglycine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C12H15FN2O2/c1-15(2)8-14-11(12(16)17-3)9-6-4-5-7-10(9)13/h4-8,11H,1-3H3

InchiKey: IOGMVOMKFFCYNH-UHFFFAOYSA-N

Formula: C12H15FN2O2

SMILES: COC(=O)C(N=CN(C)C)c1ccccc1F

Mol. weight [g/mol]: 238.26

Physical Properties

Property code	Value	Unit	Source
hf	-362.39	kJ/mol	Joback Method
hvap	58.55	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.630		Crippen Method
mcvol	181.050	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1707.00		NIST Webbook
tb	669.86	K	Joback Method
tc	882.99	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=U375811&Units=SI

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

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