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

Inchi: InChI=1S/C13H17FN2O2/c1-4-18-13(17)12(15-9-16(2)3)10-7-5-6-8-11(10)14/h5-9,12H,4

InchiKey: VKNHMWZXPJWSQC-UHFFFAOYSA-N

Formula: C13H17FN2O2

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

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	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	692.74	K	Joback Method
tc	902.72	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=U375810&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