

# p-Fluoro-L-phenylalanine, N-dimethylaminomethylene-, ethyl ester

**Inchi:** InChI=1S/C14H19FN2O2/c1-4-19-14(18)13(16-10-17(2)3)9-11-5-7-12(15)8-6-11/h5-8,10  
**InchiKey:** SQUXCQFPSHYGFL-UHFFFAOYSA-N  
**Formula:** C14H19FN2O2  
**SMILES:** CCOC(=O)C(Cc1ccc(F)cc1)N=CN(C)C  
**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	-2.32		Crippen Method
logp	1.890		Crippen Method
mcvol	209.230	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	715.62	K	Joback Method
tc	922.86	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375827&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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