

# L-Proline, N-(3-fluorobenzoyl)-, methyl ester

**Inchi:** InChI=1S/C13H14FNO3/c1-18-13(17)11-6-3-7-15(11)12(16)9-4-2-5-10(14)8-9/h2,4-5,8,1  
**InchiKey:** FDWLPRWNWHORKC-UHFFFAOYSA-N  
**Formula:** C13H14FNO3  
**SMILES:** COC(=O)C1CCCN1C(=O)c1cccc(F)c1  
**Mol. weight [g/mol]:** 251.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.603		Crippen Method
mcvol	180.170	ml/mol	McGowan Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299677&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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