

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

**Inchi:** InChI=1S/C15H18FNO3/c1-2-9-20-15(19)13-7-4-8-17(13)14(18)11-5-3-6-12(16)10-11/h3  
**InchiKey:** XRTJSYLSTFLBMG-UHFFFAOYSA-N  
**Formula:** C15H18FNO3  
**SMILES:** CCCOC(=O)C1CCCN1C(=O)c1cccc(F)c1  
**Mol. weight [g/mol]:** 279.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.383		Crippen Method
mcvol	208.350	ml/mol	McGowan Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346278&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## 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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