

# L-Proline, N-(3-chloro-2-fluorobenzoyl)-, butyl ester

**Inchi:** InChI=1S/C16H19ClFNO3/c1-2-3-10-22-16(21)13-8-5-9-19(13)15(20)11-6-4-7-12(17)14(21)  
**InchiKey:** KGBFTDMYJDPOGR-UHFFFAOYSA-N  
**Formula:** C16H19ClFNO3  
**SMILES:** CCCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F  
**Mol. weight [g/mol]:** 327.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.427		Crippen Method
mcvol	234.680	ml/mol	McGowan Method
rmpol	2372.00		NIST Webbook
rmpol	2372.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345936&Units=SI>

## Legend

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

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