

# L-Proline, N-(4-chlorobenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C18H24ClNO3/c1-2-3-4-5-13-23-18(22)16-7-6-12-20(16)17(21)14-8-10-15(19)  
**InchiKey:** AANQEDUTXPSAPD-UHFFFAOYSA-N  
**Formula:** C18H24ClNO3  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1  
**Mol. weight [g/mol]:** 337.84

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	4.068		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346149&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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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