

# L-Proline, N-(hexanoyl)-, octyl ester

**Inchi:** InChI=1S/C19H35NO3/c1-3-5-7-8-9-11-16-23-19(22)17-13-12-15-20(17)18(21)14-10-6-4  
**InchiKey:** RUDQXFDQDPKEOU-UHFFFAOYSA-N  
**Formula:** C19H35NO3  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)CCCCC  
**Mol. weight [g/mol]:** 325.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	4.461		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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=U346158&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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