

# L-Proline, N-octanoyl-, isobutyl ester

**Inchi:** InChI=1S/C17H31NO3/c1-4-5-6-7-8-11-16(19)18-12-9-10-15(18)17(20)21-13-14(2)3/h14  
**InchiKey:** JAMGRMTMFVISWKE-UHFFFAOYSA-N  
**Formula:** C17H31NO3  
**SMILES:** CCCCCCCC(=O)N1CCCC1C(=O)OCC(C)C  
**Mol. weight [g/mol]:** 297.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	3.537		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346239&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)

## 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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