

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

**Inchi:** InChI=1S/C22H41NO3/c1-3-5-7-9-10-12-14-19-26-22(25)20-16-15-18-23(20)21(24)17-18  
**InchiKey:** LTBCHHKJIRQWOW-UHFFFAOYSA-N  
**Formula:** C22H41NO3  
**SMILES:** CCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC  
**Mol. weight [g/mol]:** 367.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	5.632		Crippen Method
mcvol	328.970	ml/mol	McGowan Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346244&Units=SI>

## 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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