

# L-Proline, N-(thiophen-2-carbonyl)-, octyl ester

**Inchi:** InChI=1S/C18H27NO3S/c1-2-3-4-5-6-7-13-22-18(21)15-10-8-12-19(15)17(20)16-11-9-14  
**InchiKey:** PWQWLROLLYFVLT-UHFFFAOYSA-N  
**Formula:** C18H27NO3S  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)c1cccs1  
**Mol. weight [g/mol]:** 337.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	4.256		Crippen Method
mcvol	269.500	ml/mol	McGowan Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346374&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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