

# I-Proline, N-capryloyl-, methyl ester

**Inchi:** InChI=1S/C14H25NO3/c1-3-4-5-6-7-10-13(16)15-11-8-9-12(15)14(17)18-2/h12H,3-11H2  
**InchiKey:** PIIYQBLKPQBPRB-UHFFFAOYSA-N  
**Formula:** C14H25NO3  
**SMILES:** CCCCCC(=O)N1CCCC1C(=O)OC  
**Mol. weight [g/mol]:** 255.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.511		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299726&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)  
**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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