

# 5-Oxo-1-phenylacetyl-pyrrolidine-2-carboxylic acid methyl ester

**Other names:** 5-Oxoproline, N-(phenylacetyl), methyl ester  
**Inchi:** InChI=1S/C14H15NO4/c1-19-14(18)11-7-8-12(16)15(11)13(17)9-10-5-3-2-4-6-10/h2-6,1  
**InchiKey:** ODDCKAZQWSFWLA-UHFFFAOYSA-N  
**Formula:** C14H15NO4  
**SMILES:** COC(=O)C1CCC(=O)N1C(=O)Cc1ccccc1  
**Mol. weight [g/mol]:** 261.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	0.920		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1988.00		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=R106411&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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