

# Pyrrolidin-2-one, 1-[1-(4-carbomethoxyphenyl)butan-1-ol-2-yl]-

**Other names:** 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-oxo-dihydro-) methyl  
**Inchi:** InChI=1S/C16H21NO4/c1-3-13(17-10-4-5-14(17)18)15(19)11-6-8-12(9-7-11)16(20)21-2/  
**InchiKey:** BULBLXXKCKVDBY-UHFFFAOYSA-N  
**Formula:** C16H21NO4  
**SMILES:** CCC(C(O)c1ccc(C(=O)OC)cc1)N1CCCC1=O  
**Mol. weight [g/mol]:** 291.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.908		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		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=U360390&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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