

# 4-Methoxy-6-phenethyl-2H-pyran-2-one

**Inchi:** InChI=1S/C14H14O3/c1-16-13-9-12(17-14(15)10-13)8-7-11-5-3-2-4-6-11/h2-6,9-10H,7-8  
**InchiKey:** OVXOWIKMOIVICB-UHFFFAOYSA-N  
**Formula:** C14H14O3  
**SMILES:** COc1cc(CCc2ccccc2)oc(=O)c1  
**Mol. weight [g/mol]:** 230.26  
**CAS:** 3155-51-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	2.434		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		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=C3155519&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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