

# 4-Methyl-6-isobutyl-2-pyranone

**Inchi:** InChI=1S/C10H14O2/c1-7(2)4-9-5-8(3)6-10(11)12-9/h5-7H,4H2,1-3H3  
**InchiKey:** UGRSXCWBFZVEP-UHFFFAOYSA-N  
**Formula:** C10H14O2  
**SMILES:** Cc1cc(CC(C)C)oc(=O)c1  
**Mol. weight [g/mol]:** 166.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	2.147		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1406.00		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=R232050&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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