

# 3-hydroxy-6-methyl-2(2H)-pyranone

**Inchi:** InChI=1S/C6H6O3/c1-4-2-3-5(7)6(8)9-4/h2-3,7H,1H3  
**InchiKey:** MJIACMMODTYUHG-UHFFFAOYSA-N  
**Formula:** C6H6O3  
**SMILES:** Cc1ccc(O)c(=O)o1  
**Mol. weight [g/mol]:** 126.11

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	0.654		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2035.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R225611&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

**ripol:** Polar retention indices

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