

# 1-(5-methyl-2-furyl)-1,2-propanedione

**Inchi:** InChI=1S/C8H8O3/c1-5-3-4-7(11-5)8(10)6(2)9/h3-4H,1-2H3  
**InchiKey:** CSILYJHAPLAXTQ-UHFFFAOYSA-N  
**Formula:** C8H8O3  
**SMILES:** CC(=O)C(=O)c1ccc(C)o1  
**Mol. weight [g/mol]:** 152.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	1.360		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
ripol	1155.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1853.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=R248010&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  
**ripol:** Polar retention indices

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