

# 2-acetyl-5-formylfuran

**Inchi:** InChI=1S/C7H6O3/c1-5(9)7-3-2-6(4-8)10-7/h2-4H,1H3  
**InchiKey:** COGVGDXHVCDEAN-UHFFFAOYSA-N  
**Formula:** C7H6O3  
**SMILES:** CC(=O)c1ccc(C=O)o1  
**Mol. weight [g/mol]:** 138.12

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	1.295		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
rinpol	1118.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1116.00		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=R495360&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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