

# 2-Furancarboxylic acid, 5-(hydroxymethyl)-, methyl ester

**Inchi:** InChI=1S/C7H8O4/c1-9-6-4-3-5(11-6)7(8)10-2/h3-4H,1-2H3  
**InchiKey:** ZGQYNYHYTIYLGB-UHFFFAOYSA-N  
**Formula:** C7H8O4  
**SMILES:** COC(=O)c1ccc(OC)o1  
**Mol. weight [g/mol]:** 156.14  
**CAS:** 36802-01-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	1.075		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C36802014&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)

## 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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