

# 3-methyl-2-(2-oxopropyl)thiophene

**Inchi:** InChI=1S/C8H10OS/c1-6-3-4-10-8(6)5-7(2)9/h3-4H,5H2,1-2H3  
**InchiKey:** XDBOTNWICPQGCC-UHFFFAOYSA-N  
**Formula:** C8H10OS  
**SMILES:** CC(=O)Cc1sccc1C  
**Mol. weight [g/mol]:** 154.23

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	2.188		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
rinpol	1192.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R220121&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

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