

# 2-Butanoyl-thiazole

**Inchi:** InChI=1S/C7H9NOS/c1-2-3-6(9)7-8-4-5-10-7/h4-5H,2-3H2,1H3  
**InchiKey:** PKZQHUSSGTVETH-UHFFFAOYSA-N  
**Formula:** C7H9NOS  
**SMILES:** CCCC(=O)c1nccs1  
**Mol. weight [g/mol]:** 155.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	2.126		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R441744&Units=SI>  
**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)

## 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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