

# 1,3-Butanedione, 1-(2-thienyl)-

<b>Other names:</b>	1-(2-Thienyl)-1,3-butanedione 2-Thenoylacetone
<b>Inchi:</b>	InChI=1S/C8H8O2S/c1-6(9)5-7(10)8-3-2-4-11-8/h2-4H,5H2,1H3
<b>InchiKey:</b>	BSXCLFYNJYBVPM-UHFFFAOYSA-N
<b>Formula:</b>	C8H8O2S
<b>SMILES:</b>	CC(=O)CC(=O)c1cccs1
<b>Mol. weight [g/mol]:</b>	168.21
<b>CAS:</b>	3051-27-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	1.910		Crippen Method
mcvol	123.610	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3051272&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3051272&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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