

# 1,3-Dithienyl-2-propen-1-one

<b>Other names:</b>	1,3-di-(2-Thienyl)-2-propen-1-one 1,3-di-2-Thienyl-2-propene-1-one 2-Propen-1-one, 1,3-di-2-thienyl-
<b>Inchi:</b>	InChI=1S/C11H8OS2/c12-10(11-4-2-8-14-11)6-5-9-3-1-7-13-9/h1-8H/b6-5+
<b>InchiKey:</b>	WCAGHDMFZMUUPQ-AATRIKPKSA-N
<b>Formula:</b>	C11H8OS2
<b>SMILES:</b>	O=C(C=Cc1cccs1)c1cccs1
<b>Mol. weight [g/mol]:</b>	220.31
<b>CAS:</b>	2309-48-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	3.706		Crippen Method
mcvol	156.900	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2309480&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2309480&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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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