

# 3-[2-Methyl-(3-thienyldithio)pentan-2-one

<b>Inchi:</b>	InChI=1S/C10H14OS3/c1-4-9(7(2)11)13-14-10-5-6-12-8(10)3/h5-6,9H,4H2,1-3H3
<b>InchiKey:</b>	GCIGUMILPZYHLR-UHFFFAOYSA-N
<b>Formula:</b>	C10H14OS3
<b>SMILES:</b>	CCC(SSc1ccsc1C)C(C)=O
<b>Mol. weight [g/mol]:</b>	246.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	4.164		Crippen Method
mcvol	182.920	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R90612&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R90612&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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
<b>rinpol:</b>	Non-polar retention indices

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