

# Ketone, 5-chloro-4-nitro-2-thienyl methyl

<b>Inchi:</b>	InChI=1S/C6H4ClNO3S/c1-3(9)5-2-4(8(10)11)6(7)12-5/h2H,1H3
<b>InchiKey:</b>	HHHNIUPEIAJYKY-UHFFFAOYSA-N
<b>Formula:</b>	C6H4ClNO3S
<b>SMILES:</b>	CC(=O)c1cc([N+](=O)[O-])c(Cl)s1
<b>Mol. weight [g/mol]:</b>	205.62
<b>CAS:</b>	42456-75-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	2.512		Crippen Method
mcvol	123.520	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C42456757&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42456757&amp;Units=SI</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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