

# 1-Heptanone, 1-(2-thienyl)-

<b>Other names:</b>	2-(n-Heptanoyl)thiophene
<b>Inchi:</b>	InChI=1S/C11H16OS/c1-2-3-4-5-7-10(12)11-8-6-9-13-11/h6,8-9H,2-5,7H2,1H3
<b>InchiKey:</b>	BDNFJEMAAFFMFH-UHFFFAOYSA-N
<b>Formula:</b>	C11H16OS
<b>SMILES:</b>	CCCCCCC(=O)c1cccs1
<b>Mol. weight [g/mol]:</b>	196.31
<b>CAS:</b>	30711-40-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.901		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
ripol	1565.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2209.00		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=C30711401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C30711401&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>

## 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>ripol:</b>	Non-polar retention indices

**ripol:** Polar retention indices

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