

# 2,3,5-Trimethylthiophene

<b>Other names:</b>	Thiophene, 2,3,5-trimethyl-
<b>Inchi:</b>	InChI=1S/C7H10S/c1-5-4-6(2)8-7(5)3/h4H,1-3H3
<b>InchiKey:</b>	QKZJQIHBRCFDGQ-UHFFFAOYSA-N
<b>Formula:</b>	C7H10S
<b>SMILES:</b>	Cc1cc(C)c(C)s1
<b>Mol. weight [g/mol]:</b>	126.22
<b>CAS:</b>	1795-05-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.673		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	959.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	967.00		NIST Webbook

## 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=C1795057&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795057&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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