

# Thiophene, 2-[(1-methylethyl)thio]-

<b>Other names:</b>	2-(Isopropylthio)thiophene 2-(2-Thienyl-thio)-propane Thiophene, 2-(isopropylthio)- 2-(Isopropylsulfanyl)thiophene
<b>Inchi:</b>	InChI=1S/C7H10S2/c1-6(2)9-7-4-3-5-8-7/h3-6H,1-2H3
<b>InchiKey:</b>	INLCSHFGQRKEKW-UHFFFAOYSA-N
<b>Formula:</b>	C7H10S2
<b>SMILES:</b>	CC(C)Sc1cccs1
<b>Mol. weight [g/mol]:</b>	158.28
<b>CAS:</b>	50878-65-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	3.249		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1162.00		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=C50878654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50878654&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>rinpol:</b>	Non-polar retention indices

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