

# Triophene-2-thiol, 2-methylpropyl ether

**Other names:** 2-(isobutylsulfanyl)thiophene  
**Inchi:** InChI=1S/C8H12S2/c1-7(2)6-10-8-4-3-5-9-8/h3-5,7H,6H2,1-2H3  
**InchiKey:** JZNYNFIKHPANKO-UHFFFAOYSA-N  
**Formula:** C8H12S2  
**SMILES:** CC(C)CSc1cccs1  
**Mol. weight [g/mol]:** 172.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	3.496		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
rinpol	1249.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U395090&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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