

# Thiophene, 2-(1-methylpropyl)thio

**Inchi:** InChI=1S/C8H12S2/c1-3-7(2)10-8-5-4-6-9-8/h4-7H,3H2,1-2H3  
**InchiKey:** MGLRFPVDQZHEOJ-UHFFFAOYSA-N  
**Formula:** C8H12S2  
**SMILES:** CCC(C)Sc1cccs1  
**Mol. weight [g/mol]:** 172.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	3.639		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
rinpol	1250.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1260.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R57729&Units=SI>

## 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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