

# Thiophene, 3-(1-methylethyl)thio

**Inchi:** InChI=1S/C7H10S2/c1-6(2)9-7-3-4-8-5-7/h3-6H,1-2H3  
**InchiKey:** IUWNGVPRUJILJM-UHFFFAOYSA-N  
**Formula:** C7H10S2  
**SMILES:** CC(C)Sc1ccsc1  
**Mol. weight [g/mol]:** 158.28

## 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	1168.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1161.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R57765&Units=SI>  
**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)

## 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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