

# a-Thienothiophene

**Inchi:** InChI=1S/C8H6S2/c1-3-7(9-5-1)8-4-2-6-10-8/h1-6H  
**InchiKey:** OHZAHWOAMVVGEL-UHFFFAOYSA-N  
**Formula:** C8H6S2  
**SMILES:** c1csc(-c2cccs2)c1  
**Mol. weight [g/mol]:** 166.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.477		Crippen Method
mcvol	117.360	ml/mol	McGowan Method
rinpol	1215.00		NIST Webbook
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## 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=R640456&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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