

# Thiophene-2-thiol, S-acetyl-

**Inchi:** InChI=1S/C6H6OS2/c1-5(7)9-6-3-2-4-8-6/h2-4H,1H3  
**InchiKey:** JCCFKXLGGNMORV-UHFFFAOYSA-N  
**Formula:** C6H6OS2  
**SMILES:** CC(=O)Sc1cccs1  
**Mol. weight [g/mol]:** 158.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	2.387		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
rinpol	1264.20		NIST Webbook
rinpol	1264.20		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=U352276&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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