

# propyl 3,4-dimethyl-2-thienyl disulfide

**Inchi:** InChI=1S/C9H14S3/c1-4-5-11-12-9-8(3)7(2)6-10-9/h6H,4-5H2,1-3H3  
**InchiKey:** GQTMTKKPPSGWKQ-UHFFFAOYSA-N  
**Formula:** C9H14S3  
**SMILES:** CCCSSc1scc(C)c1C  
**Mol. weight [g/mol]:** 218.40  
**CAS:** 126876-33-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.515		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
rinpole	1663.80		NIST Webbook
rinpole	1635.00		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=C126876333&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  
**rinpole:** Non-polar retention indices

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