

# Dibenzothiophene, 1,8-dimethyl

**Other names:** 1,8-dimethyl-dibenzothiophene  
**Inchi:** InChI=1S/C14H12S/c1-9-6-7-12-11(8-9)14-10(2)4-3-5-13(14)15-12/h3-8H,1-2H3  
**InchiKey:** KMPJENUWHPZRGZ-UHFFFAOYSA-N  
**Formula:** C14H12S  
**SMILES:** Cc1ccc2sc3cccc(C)c3c2c1  
**Mol. weight [g/mol]:** 212.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Crippen Method
logp	4.671		Crippen Method
mcvol	166.090	ml/mol	McGowan Method
rinpol	335.65		NIST Webbook
rinpol	332.86		NIST Webbook
rinpol	332.86		NIST Webbook
rinpol	335.65		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=R67293&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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