

# Dibenzothiophene, 3,6-dimethyl

<b>Other names:</b>	3,6-dimethyl-dibenzothiophene
<b>Inchi:</b>	InChI=1S/C14H12S/c1-9-6-7-11-12-5-3-4-10(2)14(12)15-13(11)8-9/h3-8H,1-2H3
<b>InchiKey:</b>	JTASASABTJTWTR-UHFFFAOYSA-N
<b>Formula:</b>	C14H12S
<b>SMILES:</b>	<chem>Cc1ccc2c(c1)sc1c(C)cccc12</chem>
<b>Mol. weight [g/mol]:</b>	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	331.49		NIST Webbook
rinpol	333.44		NIST Webbook
rinpol	332.80		NIST Webbook
rinpol	332.88		NIST Webbook
rinpol	333.40		NIST Webbook
rinpol	332.90		NIST Webbook
rinpol	332.90		NIST Webbook
rinpol	332.88		NIST Webbook
rinpol	329.25		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R20964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R20964&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcpol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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