

# 3,4,6-trimethyl-dibenzothiophene

<b>Other names:</b>	Dibenzothiophene, 3,4,6-trimethyl
<b>Inchi:</b>	InChI=1S/C15H14S/c1-9-7-8-13-12-6-4-5-10(2)14(12)16-15(13)11(9)3/h4-8H,1-3H3
<b>InchiKey:</b>	YMQMZDMZBCESE-UHFFFAOYSA-N
<b>Formula:</b>	C15H14S
<b>SMILES:</b>	<chem>Cc1ccc2c(sc3c(C)cccc32)c1C</chem>
<b>Mol. weight [g/mol]:</b>	226.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.980		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
rinsol	350.52		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=R86289&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R86289&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinsol:</b>	Non-polar retention indices

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