

# 1,4,6,8-tetramethyl-dibenzothiophene

<b>Inchi:</b>	InChI=1S/C16H16S/c1-9-7-12(4)15-13(8-9)14-10(2)5-6-11(3)16(14)17-15/h5-8H,1-4H3
<b>InchiKey:</b>	MYMQFUGMSSCOAW-UHFFFAOYSA-N
<b>Formula:</b>	C16H16S
<b>SMILES:</b>	Cc1cc(C)c2sc3c(C)ccc(C)c3c2c1
<b>Mol. weight [g/mol]:</b>	240.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.74		Crippen Method
logp	5.288		Crippen Method
mcvol	194.270	ml/mol	McGowan Method
rinpol	362.34		NIST Webbook

## Sources

<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=R436034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436034&amp;Units=SI</a>
<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>

## 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>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-679-4/1-4-6-8-tetramethyl-dibenzothiophene.pdf>

Generated by Cheméo on 2024-04-26 03:34:45.854591481 +0000 UTC m=+16391734.775168793.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.