

# 2,4,6,7-tetramethyl-dibenzothiophene

<b>Inchi:</b>	InChI=1S/C16H16S/c1-9-7-11(3)15-14(8-9)13-6-5-10(2)12(4)16(13)17-15/h5-8H,1-4H3
<b>InchiKey:</b>	PGHXENCVIGQVRI-UHFFFAOYSA-N
<b>Formula:</b>	C16H16S
<b>SMILES:</b>	Cc1cc(C)c2sc3c(C)c(C)ccc3c2c1
<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
rinpola	366.40		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R436123&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436123&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

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

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