

2,4,6,8-tetramethyl-dibenzothiophene

Inchi:	InChI=1S/C16H16S/c1-9-5-11(3)15-13(7-9)14-8-10(2)6-12(4)16(14)17-15/h5-8H,1-4H3
InchiKey:	PWZYSQKXNQYCFX-UHFFFAOYSA-N
Formula:	C16H16S
SMILES:	Cc1cc(C)c2sc3c(C)cc(C)cc3c2c1
Mol. weight [g/mol]:	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	359.69		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	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=R436138&Units=SI

Legend

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

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