2,4,6,7-tetramethyl-dibenzothiophene

Inchi: 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
InchiKey: PGHXENCVIGQVRI-UHFFFAOYSA-N
Formula: C16H16S
SMILES: Cc1cc(C)c2sc3c(C)c(C)ccc3c2c1
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
rinpol	366.40		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R436123&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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