1,2,4-trimethyl-dibenzothiophene

Inchi: InChI=1S/C15H14S/c1-9-8-10(2)15-14(11(9)3)12-6-4-5-7-13(12)16-15/h4-8H,1-3H3
InchiKey: JNDTZHLOQBQHLS-UHFFFAOYSA-N
Formula: C15H14S
SMILES: Cc1cc(C)c2sc3ccccc3c2c1C
Mol. weight [g/mol]: 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
rinpol	357.30		NIST Webbook

Sources

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=R435997&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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