1,3,7-trimethyl-dibenzothiophene

Other names: Dibenzothiophene, 1,3,7-trimethyl
Inchi: InChI=1S/C15H14S/c1-9-4-5-12-13(7-9)16-14-8-10(2)6-11(3)15(12)14/h4-8H,1-3H3
InchiKey: RTYGEGPUDNKTKI-UHFFFAOYSA-N
Formula: C15H14S
SMILES: Cc1ccc2c(c1)sc1cc(C)cc(C)c12
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	2208.00		NIST Webbook
rinpol	354.34		NIST Webbook
rinpol	352.37		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=R192977&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

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