1,9-dimethyl-dibenzothiophene

Other names: Dibenzothiophene, 1,9-dimethyl
Inchi: InChI=1S/C14H12S/c1-9-5-3-7-11-13(9)14-10(2)6-4-8-12(14)15-11/h3-8H,1-2H3
InchiKey: DGUACJDPTAAFMP-UHFFFAOYSA-N
Formula: C14H12S
SMILES: Cc1cccc2sc3cccc(C)c3c12
Mol. weight [g/mol]: 212.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Crippen Method
logp	4.671		Crippen Method
mcvol	166.090	ml/mol	McGowan Method
rinpol	339.49		NIST Webbook
rinpol	339.49		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R67300&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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