Dibenzothiophene, 1,6-dimethyl

Inchi: InChI=1S/C14H12S/c1-9-5-4-8-12-13(9)11-7-3-6-10(2)14(11)15-12/h3-8H,1-2H3
InchiKey: KCDDLWLZPFIOGI-UHFFFAOYSA-N
Formula: C14H12S
SMILES: Cc1cccc2c1sc1cccc(C)c12
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	332.80		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R67261&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