1,3-Dimethyldibenzothiophene

Other names: Dibenzothiophene, 1,3-dimethyl
Inchi: InChI=1S/C14H12S/c1-9-7-10(2)14-11-5-3-4-6-12(11)15-13(14)8-9/h3-8H,1-2H3
InchiKey: IPMMDFNYBNKMQS-UHFFFAOYSA-N
Formula: C14H12S
SMILES: Cc1cc(C)c2c(c1)sc1ccccc12
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	336.65		NIST Webbook
rinpol	334.73		NIST Webbook
rinpol	2079.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383550&Units=SI

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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