Dibenzothiophene, 3,4-dimethyl

Other names: 3,4-dimethyl-dibenzothiophene
Inchi: InChI=1S/C14H12S/c1-9-7-8-12-11-5-3-4-6-13(11)15-14(12)10(9)2/h3-8H,1-2H3
InchiKey: BRZWYUOAWQYIAT-UHFFFAOYSA-N
Formula: C14H12S
SMILES: Cc1ccc2c(sc3ccccc32)c1C
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	336.80		NIST Webbook
rinpol	335.09		NIST Webbook
rinpol	335.10		NIST Webbook
rinpol	334.60		NIST Webbook
rinpol	336.34		NIST Webbook
rinpol	336.34		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R67289&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