2,3,4-trimethyl-benzothiophene

Other names: Benzothiophene, 2,3,4-trimethyl
Inchi: InChI=1S/C11H12S/c1-7-5-4-6-10-11(7)8(2)9(3)12-10/h4-6H,1-3H3
InchiKey: GTMJIBWPIOYZSG-UHFFFAOYSA-N
Formula: C11H12S
SMILES: Cc1sc2cccc(C)c2c1C
Mol. weight [g/mol]: 176.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.827		Crippen Method
mcvol	143.280	ml/mol	McGowan Method
rinpol	260.30		NIST Webbook
rinpol	260.30		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R85956&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