

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:	GTMJIBWPLOYZSG-UHFFFAOYSA-N
Formula:	C11H12S
SMILES:	<chem>Cc1sc2cccc(C)c2c1C</chem>
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

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