

Benzo[b]thiophene, 2,5,7-trimethyl-

Other names:	Benzothiophene, 2,5,7-trimethyl
Inchi:	InChI=1S/C11H12S/c1-7-4-8(2)11-10(5-7)6-9(3)12-11/h4-6H,1-3H3
InchiKey:	PNEAISMECMOVFA-UHFFFAOYSA-N
Formula:	C11H12S
SMILES:	<chem>Cc1cc(C)c2sc(C)cc2c1</chem>
Mol. weight [g/mol]:	176.28
CAS:	16587-65-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.827		Crippen Method
mcvol	143.280	ml/mol	McGowan Method
rinpola	1593.00		NIST Webbook
rinpola	1593.00		NIST Webbook

Sources

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=C16587658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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