

Benzo[b]thiophene, 3,5-dimethyl-

Other names:	3,5-Dimethylbenzo[b]thiophene 3,5-dimethy-benzothiophene
Inchi:	InChI=1S/C10H10S/c1-7-3-4-10-9(5-7)8(2)6-11-10/h3-6H,1-2H3
InchiKey:	UQJSHXYNNVEGMQ-UHFFFAOYSA-N
Formula:	C10H10S
SMILES:	Cc1ccc2scc(C)c2c1
Mol. weight [g/mol]:	162.25
CAS:	1964-45-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.518		Crippen Method
mcvol	129.190	ml/mol	McGowan Method
rinpol	243.40		NIST Webbook
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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=C1964450&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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