

Benzo[b]thiophene, 2,5-dimethyl-

Other names:	Benzothiophene, 2,5-dimethyl
Inchi:	InChI=1S/C10H10S/c1-7-3-4-10-9(5-7)6-8(2)11-10/h3-6H,1-2H3
InchiKey:	FJPNWMZUNBSFIQ-UHFFFAOYSA-N
Formula:	C10H10S
SMILES:	<chem>Cc1ccc2sc(C)cc2c1</chem>
Mol. weight [g/mol]:	162.25
CAS:	16587-48-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.518		Crippen Method
mcvol	129.190	ml/mol	McGowan Method

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=C16587487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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