

Benzo[b]thiophene, 6-methyl-

Other names:	6-Methylbenzo[b]thiophene 6-Methylthianaphthene 6-Methyl-1-benzothiophene 6-Methyl-benzothiophene Benzothiophene, 6-methyl
Inchi:	InChI=1S/C9H8S/c1-7-2-3-8-4-5-10-9(8)6-7/h2-6H,1H3
InchiKey:	WOGMIMNVXACKEB-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	Cc1ccc2ccsc2c1
Mol. weight [g/mol]:	148.22
CAS:	16587-47-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	3.210		Crippen Method
mcvol	115.100	ml/mol	McGowan Method
rinpol	222.00		NIST Webbook
rinpol	222.11		NIST Webbook
rinpol	214.77		NIST Webbook

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=C16587476&Units=SI

Legend

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

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