

Benzo[b]thiophene, 5-methyl-

Other names:	5-Methylbenzo[b]thiophene 5-Methyl-1-benzothiophene 5-Methyl-benzothiophene Benzothiophene, 5-methyl
Inchi:	InChI=1S/C9H8S/c1-7-2-3-9-8(6-7)4-5-10-9/h2-6H,1H3
InchiKey:	DOHZWDWNQFZIKH-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	Cc1ccc2sccc2c1
Mol. weight [g/mol]:	148.22
CAS:	14315-14-1

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	221.81		NIST Webbook
rinpol	222.00		NIST Webbook
rinpol	222.09		NIST Webbook
rinpol	214.77		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14315141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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