

Benzo[b]thiophene, 4-methyl-

Other names:	4-Methylbenzo[b]thiophene 4-Methylbenzothiophene Benzothiophene, 4-methyl
Inchi:	InChI=1S/C9H8S/c1-7-3-2-4-9-8(7)5-6-10-9/h2-6H,1H3
InchiKey:	RPKWIZPGQZKQKY-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	Cc1cccc2sccc12
Mol. weight [g/mol]:	148.22
CAS:	14315-11-8

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	223.10		NIST Webbook
rinpol	223.15		NIST Webbook
rinpol	215.59		NIST Webbook
rinpol	215.59		NIST Webbook
rinpol	223.15		NIST Webbook
rinpol	223.15		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=C14315118&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
rinpol: Non-polar retention indices

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