

Benzo[b]thiophene, 7-methyl

Other names:	7-methyl-benzothiophene 7-Methylbenzo[b]thiophene Benzothiophene, 7-methyl
Inchi:	InChI=1S/C9H8S/c1-7-3-2-4-8-5-6-10-9(7)8/h2-6H,1H3
InchiKey:	PIHVNUSWMTZFBD-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	Cc1cccc2ccsc12
Mol. weight [g/mol]:	148.22

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	212.61		NIST Webbook
rinpol	212.61		NIST Webbook
rinpol	219.10		NIST Webbook
rinpol	219.10		NIST Webbook
rinpol	219.20		NIST Webbook
rinpol	219.16		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21023&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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