

3-Methylbenzothiophene

Other names:	3-Methylbenzo[b]thiophene Benzo[b]thiophene, 3-methyl- Benzothiophene, 3-methyl- 3-Methyl-1-thiaindene 3-Methylthianaphthene 3-Methylthioindene
Inchi:	InChI=1S/C9H8S/c1-7-6-10-9-5-3-2-4-8(7)9/h2-6H,1H3
InchiKey:	SEBRPHZZSLCDRQ-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	<chem>Cc1csc2ccccc12</chem>
Mol. weight [g/mol]:	148.22
CAS:	1455-18-1

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	215.59		NIST Webbook
rinpol	223.08		NIST Webbook
rinpol	221.02		NIST Webbook
rinpol	224.68		NIST Webbook
rinpol	223.10		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	215.59		NIST Webbook
rinpol	223.10		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1315.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1455181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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