Benzo[b]thiophene, 2-methyl-

Other names:	2-Methyl-1-thiaindene
	2-Methylbenzothiophene
	2-Methylbenzo(b)thiophene
	2-Methylthianaphthene
	2-Methylthioindene
	Benzothiophene, 2-methyl
Inchi:	InChI=1S/C9H8S/c1-7-6-8-4-2-3-5-9(8)10-7/h2-6H,1H3
InchiKey:	BLZKSRBAQDZAIX-UHFFFAOYSA-N
Formula:	C9H8S
SMILES:	Cc1cc2ccccc2s1
Mol. weight [g/mol]:	148.22
CAS:	1195-14-8

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	220.45		NIST Webbook
rinpol	221.00		NIST Webbook
rinpol	220.76		NIST Webbook
rinpol	218.74		NIST Webbook
rinpol	213.78		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1195148&Units=SI
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

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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