

# Benzo[b]thiophene, 2-methyl-

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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1195148&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1195148&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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