

# 1-Methyldibenzothiophene

<b>Other names:</b>	Dibenzo[b]thiophene, 1-methyl Dibenzothiophene, 1-methyl
<b>Inchi:</b>	InChI=1S/C13H10S/c1-9-5-4-8-12-13(9)10-6-2-3-7-11(10)14-12/h2-8H,1H3
<b>InchiKey:</b>	HORCQSAKJDDDBKB-UHFFFAOYSA-N
<b>Formula:</b>	C13H10S
<b>SMILES:</b>	Cc1cccc2sc3ccccc3c12
<b>Mol. weight [g/mol]:</b>	198.28
<b>CAS:</b>	31317-07-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	4.363		Crippen Method
mccvol	152.000	ml/mol	McGowan Method
rinpol	319.22		NIST Webbook
rinpol	319.22		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	319.35		NIST Webbook
rinpol	318.68		NIST Webbook
rinpol	318.65		NIST Webbook
rinpol	310.67		NIST Webbook
rinpol	319.35		NIST Webbook
rinpol	319.75		NIST Webbook
rinpol	318.80		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	319.69		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	317.10		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	318.22		NIST Webbook
rinpol	319.20		NIST Webbook
rinpol	319.60		NIST Webbook

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<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=C31317074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31317074&amp;Units=SI</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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