

# Dibenzothiophene, 3-methyl-

<b>Other names:</b>	3-Methyldibenzo[b,d]thiophene 3-Methyldibenzothiophene
<b>Inchi:</b>	InChI=1S/C13H10S/c1-9-6-7-11-10-4-2-3-5-12(10)14-13(11)8-9/h2-8H,1H3
<b>InchiKey:</b>	URUCEYZTJIJMLX-UHFFFAOYSA-N
<b>Formula:</b>	C13H10S
<b>SMILES:</b>	<chem>Cc1ccc2c(c1)sc1cccc12</chem>
<b>Mol. weight [g/mol]:</b>	198.28
<b>CAS:</b>	16587-52-3

## 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	316.20		NIST Webbook
rinpol	315.68		NIST Webbook
rinpol	315.17		NIST Webbook
rinpol	315.51		NIST Webbook
rinpol	313.83		NIST Webbook
rinpol	313.83		NIST Webbook
rinpol	315.43		NIST Webbook
rinpol	315.10		NIST Webbook
rinpol	315.57		NIST Webbook
rinpol	316.72		NIST Webbook
rinpol	315.70		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	316.32		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	313.98		NIST Webbook
rinpol	313.90		NIST Webbook
rinpol	313.90		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	314.61		NIST Webbook
rinpol	316.32		NIST Webbook
rinpol	315.70		NIST Webbook
rinpol	315.80		NIST Webbook

rinpol	316.20	NIST Webbook
rinpol	316.00	NIST Webbook
rinpol	314.61	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=C16587523&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587523&amp;Units=SI</a>
<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>

## 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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