

# 2-methyl-3-thiophenethiol

<b>Other names:</b>	2-methyl-3-thiophenethiol Thiophen-3-thiol, 2-methyl 3-Thiophenethiol, 2-methyl 3-Thiophenethiol, 2-methyl- 2-Methyl-thiopene-3-thiol 2-Methylthiophen-3-thiol 2-methylthiophene-3-thiol
<b>Inchi:</b>	InChI=1S/C5H6S2/c1-4-5(6)2-3-7-4/h2-3,6H,1H3
<b>InchiKey:</b>	AQXLMAYNBMTBHD-UHFFFAOYSA-N
<b>Formula:</b>	C5H6S2
<b>SMILES:</b>	Cc1sccc1S
<b>Mol. weight [g/mol]:</b>	130.23
<b>CAS:</b>	2527-76-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	2.345		Crippen Method
mcvol	94.550	ml/mol	McGowan Method
rinpol	1070.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook

ripol	1034.00	NIST Webbook
ripol	1066.00	NIST Webbook
ripol	1584.00	NIST Webbook
ripol	1559.00	NIST Webbook
ripol	1559.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1559.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C2527766&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2527766&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>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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