

# 3-Thiophenethiol

<b>Other names:</b>	2-Thienyl mercaptan 3-Thienyl hydrosulfide 3-Thienyl mercaptan Thiophen-3-thiol Thiophene-3-thiol
<b>Inchi:</b>	InChI=1S/C4H4S2/c5-4-1-2-6-3-4/h1-3,5H
<b>InchiKey:</b>	VSGXHZUTTFLSBC-UHFFFAOYSA-N
<b>Formula:</b>	C4H4S2
<b>SMILES:</b>	Sc1ccsc1
<b>Mol. weight [g/mol]:</b>	116.20
<b>CAS:</b>	7774-73-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	2.037		Crippen Method
mcvol	80.460	ml/mol	McGowan Method
rinpol	944.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	954.00		NIST Webbook

ripol	1555.00	NIST Webbook
ripol	1581.00	NIST Webbook
ripol	1547.00	NIST Webbook
ripol	1547.00	NIST Webbook

## Sources

<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=C7774734&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7774734&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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
<b>ripol:</b>	Polar retention indices

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