

# Thieno[3,4-b]thiophene

<b>Other names:</b>	1,5-Thiophthene
<b>Inchi:</b>	InChI=1S/C6H4S2/c1-2-8-6-4-7-3-5(1)6/h1-4H
<b>InchiKey:</b>	PFZLGKHSYILJTH-UHFFFAOYSA-N
<b>Formula:</b>	C6H4S2
<b>SMILES:</b>	c1cc2csc2s1
<b>Mol. weight [g/mol]:</b>	140.23
<b>CAS:</b>	250-65-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	2.963		Crippen Method
mcvol	93.480	ml/mol	McGowan Method
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1975.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C250657&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C250657&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>
<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>

## 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

**ripol:** Polar retention indices

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