

# Thiophene, 2-(butylthio)-

<b>Other names:</b>	2-(Butylthio)-thiophene 2-(Butylsulfanyl)thiophene
<b>Inchi:</b>	InChI=1S/C8H12S2/c1-2-3-6-9-8-5-4-7-10-8/h4-5,7H,2-3,6H2,1H3
<b>InchiKey:</b>	PTTSDBWFNLNXII-UHFFFAOYSA-N
<b>Formula:</b>	C8H12S2
<b>SMILES:</b>	CCCCSc1cccs1
<b>Mol. weight [g/mol]:</b>	172.31
<b>CAS:</b>	3988-71-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	3.640		Crippen Method
mcpol	136.820	ml/mol	McGowan Method
rinpol	1290.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1290.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3988714&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3988714&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>rinpolar:</b>	Non-polar retention indices

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