

# 4-(2-Thienyl)butyric acid

<b>Other names:</b>	«gamma»-(«alpha»-Thienyl)butyric acid 2-Thiophenebutanoic acid 2-Thiophenebutyric acid
<b>Inchi:</b>	InChI=1S/C8H10O2S/c9-8(10)5-1-3-7-4-2-6-11-7/h2,4,6H,1,3,5H2,(H,9,10)
<b>InchiKey:</b>	VYTXLSQVYGNWLV-UHFFFAOYSA-N
<b>Formula:</b>	C8H10O2S
<b>SMILES:</b>	O=C(O)CCCc1cccs1
<b>Mol. weight [g/mol]:</b>	170.23
<b>CAS:</b>	4653-11-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	2.155		Crippen Method
mcvol	127.910	ml/mol	McGowan Method

## 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=C4653116&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4653116&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>

## 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

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