

# 5-(2-Thienoyl)butyric acid

<b>Inchi:</b>	InChI=1S/C9H10O3S/c10-7(3-1-5-9(11)12)8-4-2-6-13-8/h2,4,6H,1,3,5H2,(H,11,12)
<b>InchiKey:</b>	GSQMRVFOHNXKOR-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O3S
<b>SMILES:</b>	O=C(O)CCCC(=O)c1cccs1
<b>Mol. weight [g/mol]:</b>	198.24
<b>CAS:</b>	22971-62-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	2.186		Crippen Method
mcvol	143.570	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22971626&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22971626&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

Latest version available from:

<https://www.chemeo.com/cid/41-535-2/5-2-Thienoyl-butyric-acid.pdf>

Generated by Cheméo on 2024-04-20 08:59:56.945839229 +0000 UTC m=+15892845.866416550.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.