

# Sarcosine, N-(2-thiophenylacetyl)-, propyl ester

<b>Inchi:</b>	InChI=1S/C12H17NO3S/c1-3-6-16-12(15)9-13(2)11(14)8-10-5-4-7-17-10/h4-5,7H,3,6,8-9
<b>InchiKey:</b>	PFGUSPIYQHITED-UHFFFAOYSA-N
<b>Formula:</b>	C12H17NO3S
<b>SMILES:</b>	CCCOC(=O)CN(C)C(=O)Cc1cccs1
<b>Mol. weight [g/mol]:</b>	255.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.702		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpole	2021.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321361&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321361&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>
<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>rinpole:</b>	Non-polar retention indices

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