

# L-Serine, N,O-bis(2-thienylcarbonyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C14H13NO5S2/c1-19-13(17)9(15-12(16)10-4-2-6-21-10)8-20-14(18)11-5-3-7-2
<b>InchiKey:</b>	QNFWDFUVLGOAOB-UHFFFAOYSA-N
<b>Formula:</b>	C14H13NO5S2
<b>SMILES:</b>	COC(=O)C(COC(=O)c1cccs1)NC(=O)c1cccs1
<b>Mol. weight [g/mol]:</b>	339.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	1.938		Crippen Method
mcvol	228.330	ml/mol	McGowan Method
rinsol	2705.00		NIST Webbook
rinsol	2705.00		NIST Webbook

## Sources

<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=U299599&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299599&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinsol:</b>	Non-polar retention indices

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