

Sarcosine, N-(2-thienylcarbonyl)-, propyl ester

Inchi:	InChI=1S/C11H15NO3S/c1-3-6-15-10(13)8-12(2)11(14)9-5-4-7-16-9/h4-5,7H,3,6,8H2,1-2
InchiKey:	DWVLMOBDEBOTQB-UHFFFAOYSA-N
Formula:	C11H15NO3S
SMILES:	CCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]:	241.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.773		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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