

L-Phenylalanine, N-(2-thienylcarbonyl)-, methyl ester

Inchi:	InChI=1S/C15H15NO3S/c1-19-15(18)12(10-11-6-3-2-4-7-11)16-14(17)13-8-5-9-20-13/h2
InchiKey:	LIWKGUIEIXQWPB-UHFFFAOYSA-N
Formula:	C15H15NO3S
SMILES:	COC(=O)C(Cc1ccccc1)NC(=O)c1cccs1
Mol. weight [g/mol]:	289.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.262		Crippen Method
mcvol	214.330	ml/mol	McGowan Method
rinpola	2241.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/63-760-8/l-Phenylalanine-N-2-thienylcarbonyl-methyl-ester.pdf>

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