

«beta»-Alanine, N-(thiophene-2-carbonyl)-, propyl ester

Inchi:	InChI=1S/C11H15NO3S/c1-2-7-15-10(13)5-6-12-11(14)9-4-3-8-16-9/h3-4,8H,2,5-7H2,1H
InchiKey:	CTVHETOTZAHOOT-UHFFFAOYSA-N
Formula:	C11H15NO3S
SMILES:	CCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	241.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.821		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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