

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

Inchi:	InChI=1S/C13H19NO3S/c1-2-3-4-9-17-12(15)7-8-14-13(16)11-6-5-10-18-11/h5-6,10H,2-
InchiKey:	DDDYLVBGHPCUEX-UHFFFAOYSA-N
Formula:	C13H19NO3S
SMILES:	CCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	269.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.601		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		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=U321796&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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