

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

Inchi:	InChI=1S/C14H21NO3S/c1-2-3-4-5-10-18-13(16)8-9-15-14(17)12-7-6-11-19-12/h6-7,11H
InchiKey:	YUQVKOSQAJLICZ-UHFFFAOYSA-N
Formula:	C14H21NO3S
SMILES:	CCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	283.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	2.991		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
rinsol	2330.00		NIST Webbook
rinsol	2330.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321797&amp;Units=SI</a>

## Legend

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

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