

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

Inchi:	InChI=1S/C15H23NO3S/c1-2-3-4-5-6-11-19-14(17)9-10-16-15(18)13-8-7-12-20-13/h7-8,
InchiKey:	VBTPZICVVMMEKL-UHFFFAOYSA-N
Formula:	C15H23NO3S
SMILES:	CCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	297.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.382		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
rinpola	2435.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321798&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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