

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

Inchi:	InChI=1S/C22H37NO3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-26-21(24)16-17-23-22(25)20
InchiKey:	JYLDGWQKLHIOBC-UHFFFAOYSA-N
Formula:	C22H37NO3S
SMILES:	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	395.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.13		Crippen Method
logp	6.112		Crippen Method
mcvol	336.720	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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