

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

Inchi:	InChI=1S/C23H39NO3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-27-22(25)17-18-24-23(26)
InchiKey:	SFRZJNJOUOKRRD-UHFFFAOYSA-N
Formula:	C23H39NO3S
SMILES:	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	409.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.55		Crippen Method
logp	6.502		Crippen Method
mcvol	350.810	ml/mol	McGowan Method

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=U321805&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

Latest version available from:

<https://www.chemeo.com/cid/113-730-5/beta-Alanine-N-thiophene-2-carbonyl-pentadecyl-ester.pdf>

Generated by Cheméo on 2024-04-28 04:22:55.840511157 +0000 UTC m=+16567424.761088473.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.