«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: CCCCCCCCCCCCCCCOC(=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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume