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

Inchi: InChI=1S/C19H31NO3S/c1-2-3-4-5-6-7-8-9-10-15-23-18(21)13-14-20-19(22)17-12-11-16

InchiKey: PPNHLIUVWDYZDF-UHFFFAOYSA-N

Formula: C19H31NO3S

SMILES: CCCCCCCCCCCOC(=O)CCNC(=O)c1cccs1

Mol. weight [g/mol]: 353.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.942		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
rinpol	2889.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U321802&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices