Sarcosine, N-(2-thienylcarbonyl)-, undecyl ester

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

InchiKey: CNWALIJDAOCYFT-UHFFFAOYSA-N

Formula: C19H31NO3S

SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccs1

Mol. weight [g/mol]: 353.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.894		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
rinpol	2767.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321472&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

rinpol: Non-polar retention indices