Sarcosine, N-(2-thiophenylacetyl)-, dodecyl ester

Inchi: InChI=1S/C21H35NO3S/c1-3-4-5-6-7-8-9-10-11-12-15-25-21(24)18-22(2)20(23)17-19-14

InchiKey: QSXRHNMEFCWPRI-UHFFFAOYSA-N

Formula: C21H35NO3S

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)Cc1cccs1

Mol. weight [g/mol]: 381.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	5.213		Crippen Method
mcvol	322.630	ml/mol	McGowan Method
rinpol	3019.00		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=U321370&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