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

Inchi: InChI=1S/C20H33NO3S/c1-3-4-5-6-7-8-9-10-11-14-24-20(23)17-21(2)19(22)16-18-13-12

InchiKey: PUKWCCWALLCTRB-UHFFFAOYSA-N

Formula: C20H33NO3S

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

Mol. weight [g/mol]: 367.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	4.823		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		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=U321369&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

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