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

Inchi: InChI=1S/C16H25NO3S/c1-3-4-5-6-7-10-20-16(19)13-17(2)15(18)12-14-9-8-11-21-14/h8

InchiKey: OBUMPUGNUFRZIG-UHFFFAOYSA-N

Formula: C16H25NO3S

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

Mol. weight [g/mol]: 311.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	3.263		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		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=U321366&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.