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

Inchi: InChI=1S/C14H21NO3S/c1-3-4-5-8-18-14(17)11-15(2)13(16)10-12-7-6-9-19-12/h6-7,9H,

InchiKey: CEDVHNCBQONVGZ-UHFFFAOYSA-N

Formula: C14H21NO3S

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

Mol. weight [g/mol]: 283.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	2.482		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		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=U321364&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.