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

Inchi: InChI=1S/C13H19NO3S/c1-3-4-5-8-17-12(15)10-14(2)13(16)11-7-6-9-18-11/h6-7,9H,3-5
InchiKey: UDZMDURKHGLMGL-UHFFFAOYSA-N
Formula: C13H19NO3S
SMILES: CCCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 269.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.553		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
rinpol	2138.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321465&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