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

Inchi: InChI=1S/C15H23NO3S/c1-3-4-5-6-7-10-19-14(17)12-16(2)15(18)13-9-8-11-20-13/h8-9,
InchiKey: FJOOOQCDQXVOAE-UHFFFAOYSA-N
Formula: C15H23NO3S
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 297.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	3.334		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321468&Units=SI
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

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.