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

Inchi: InChI=1S/C11H15NO3S/c1-3-15-11(14)8-12(2)10(13)7-9-5-4-6-16-9/h4-6H,3,7-8H2,1-2H
InchiKey: FCXCXFGVLWYOHB-UHFFFAOYSA-N
Formula: C11H15NO3S
SMILES: CCOC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]: 241.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	1.312		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		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=U321360&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

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