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

Inchi: InChI=1S/C10H13NO3S/c1-3-14-9(12)7-11(2)10(13)8-5-4-6-15-8/h4-6H,3,7H2,1-2H3
InchiKey: WIWARIRWHPSDOJ-UHFFFAOYSA-N
Formula: C10H13NO3S
SMILES: CCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 227.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	1.383		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook

Sources

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=U321461&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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