Glycine, N-(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C8H9NO3S/c1-12-7(10)5-9-8(11)6-3-2-4-13-6/h2-4H,5H2,1H3,(H,9,11)
InchiKey: GCYJJPOBYJQNHH-UHFFFAOYSA-N
Formula: C8H9NO3S
SMILES: COC(=O)CNC(=O)c1cccs1
Mol. weight [g/mol]: 199.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.27		Crippen Method
logp	0.651		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
rinpol	1674.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299602&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