

L-Alanine, N-(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C9H11NO3S/c1-6(9(12)13-2)10-8(11)7-4-3-5-14-7/h3-6H,1-2H3,(H,10,11)
InchiKey: RGWBJRKEIGMOOW-UHFFFAOYSA-N
Formula: C9H11NO3S
SMILES: COC(=O)C(C)NC(=O)c1cccs1
Mol. weight [g/mol]: 213.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.039		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299594&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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