l-Proline, N-(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C11H13NO3S/c1-15-11(14)8-4-2-6-12(8)10(13)9-5-3-7-16-9/h3,5,7-8H,2,4,6H2
InchiKey: YUXRIDLDZUUCFX-UHFFFAOYSA-N
Formula: C11H13NO3S
SMILES: COC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 239.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	1.526		Crippen Method
mcvol	170.870	ml/mol	McGowan Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		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=U299596&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.