L-Proline, N-(cyclopropylcarbonyl)-, ethyl ester

Inchi: InChI=1S/C11H17NO3/c1-2-15-11(14)9-4-3-7-12(9)10(13)8-5-6-8/h8-9H,2-7H2,1H3
InchiKey: KLAZLOQZZRDANR-UHFFFAOYSA-N
Formula: C11H17NO3
SMILES: CCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	0.951		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346308&Units=SI
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

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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