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

Inchi: InChI=1S/C12H19NO3/c1-2-8-16-12(15)10-4-3-7-13(10)11(14)9-5-6-9/h9-10H,2-8H2,1H
InchiKey: VTFCIKFSHHPUDA-UHFFFAOYSA-N
Formula: C12H19NO3
SMILES: CCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]: 225.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	1.341		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
rinpol	1798.00		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=U346309&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