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

Inchi: InChI=1S/C20H35NO3/c1-2-3-4-5-6-7-8-9-10-16-24-20(23)18-12-11-15-21(18)19(22)17-
InchiKey: SQRCVZRYIHGHFO-UHFFFAOYSA-N
Formula: C20H35NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]: 337.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.461		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346318&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

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