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

Inchi: InChI=1S/C22H39NO3/c1-2-3-4-5-6-7-8-9-12-18-26-22(25)20-16-13-17-23(20)21(24)19-
InchiKey: IEDSTRSITMZZMR-UHFFFAOYSA-N
Formula: C22H39NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)C1CCCC1
Mol. weight [g/mol]: 365.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	5.242		Crippen Method
mcvol	318.110	ml/mol	McGowan Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook

Sources

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=U346107&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.