L-Proline, N-(3-phenylpropionyl)-, undecyl ester

Inchi: InChI=1S/C25H39NO3/c1-2-3-4-5-6-7-8-9-13-21-29-25(28)23-17-14-20-26(23)24(27)19-
InchiKey: DBUFRBPFHMMVFU-UHFFFAOYSA-N
Formula: C25H39NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCc1ccccc1
Mol. weight [g/mol]: 401.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	5.684		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
rinpol	3179.00		NIST Webbook
rinpol	3179.00		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=U346392&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.