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

Inchi: InChI=1S/C22H41NO3/c1-3-5-7-8-9-10-11-12-14-19-26-22(25)20-16-15-18-23(20)21(24)17-13-6-4-2
InchiKey: ZHZWELSFMHFLOX-UHFFFAOYSA-N
Formula: C22H41NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]: 367.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	5.632		Crippen Method
mcvol	328.970	ml/mol	McGowan Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346161&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

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