

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

Inchi: InChI=1S/C23H35NO3/c1-2-3-4-5-6-7-11-19-27-23(26)21-15-12-18-24(21)22(25)17-16-2
InchiKey: ZGXRYWKAWPTZGH-UHFFFAOYSA-N
Formula: C23H35NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)CCc1ccccc1
Mol. weight [g/mol]: 373.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.904		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
rinpol	2948.00		NIST Webbook
rinpol	2948.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U346390&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

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<https://www.chemeo.com/cid/99-173-1/L-Proline-N-3-phenylpropionyl-nonyl-ester.pdf>

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