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

Inchi: InChI=1S/C24H37NO3/c1-3-4-5-6-7-8-9-10-11-18-28-24(27)22-16-13-17-25(22)23(26)21
InchiKey: UOPDPITYWDQPPU-UHFFFAOYSA-N
Formula: C24H37NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	5.674		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346261&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

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