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

Inchi: InChI=1S/C25H39NO3/c1-3-4-5-6-7-8-9-10-11-12-19-29-25(28)23-17-14-18-26(23)24(27
InchiKey: ZMOSTXRSZMEZAV-UHFFFAOYSA-N
Formula: C25H39NO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 401.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	6.064		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
rinpol	3161.00		NIST Webbook
rinpol	3161.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346262&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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