

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

Inchi: InChI=1S/C22H33NO4/c1-3-4-5-6-7-8-9-16-27-22(25)20-14-11-15-23(20)21(24)18-12-10
InchiKey: CXKIWHYZZKHWQM-UHFFFAOYSA-N
Formula: C22H33NO4
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 375.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	4.594		Crippen Method
mcvol	311.080	ml/mol	McGowan Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		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=U346172&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/96-014-0/L-Proline-N-3-methoxybenzoyl-nonyl-ester.pdf>

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