

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

Inchi: InChI=1S/C22H33NO3/c1-3-4-5-6-7-8-9-16-26-22(25)20-14-11-15-23(20)21(24)19-13-10
InchiKey: PKMDUDXHIRZRGH-UHFFFAOYSA-N
Formula: C22H33NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 359.50

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.98 | | Crippen Method |
| logp | 4.893 | | Crippen Method |
| mcvol | 305.210 | ml/mol | McGowan Method |
| rinpol | 2824.00 | | NIST Webbook |
| rinpol | 2824.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346259&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/95-995-3/L-Proline-N-3-methylbenzoyl-nonyl-ester.pdf>

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