

# L-Proline, N-(3-methylbenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C19H27NO3/c1-14(2)7-6-12-23-19(22)17-10-5-11-20(17)18(21)16-9-4-8-15(3)  
**InchiKey:** CNQWUGSQDTZTNH-UHFFFAOYSA-N  
**Formula:** C19H27NO3  
**SMILES:** Cc1cccc(C(=O)N2CCCC2C(=O)OCCCC(C)C)c1  
**Mol. weight [g/mol]:** 317.42

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.49   |        | Crippen Method |
| logp          | 3.579   |        | Crippen Method |
| mcvol         | 262.940 | ml/mol | McGowan Method |
| rinpol        | 2478.00 |        | NIST Webbook   |
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## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=U346255&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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