# L-Proline, N-(3-phenylpropionyl)-, octyl ester

**Inchi:** InChI=1S/C22H33NO3/c1-2-3-4-5-6-10-18-26-22(25)20-14-11-17-23(20)21(24)16-15-19-
**InchiKey:** RGKVODVDVZXQER-UHFFFAOYSA-N
**Formula:** C22H33NO3
**SMILES:** CCCCCCCCOC(=O)C1CCCN1C(=O)CCc1ccccc1
**Mol. weight [g/mol]:** 359.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.35 | | Crippen Method |
| logp | 4.514 | | Crippen Method |
| mcvol | 305.210 | ml/mol | McGowan Method |
| rinpol | 2836.00 | | NIST Webbook |
| rinpol | 2836.00 | | NIST Webbook |

## Sources

**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=U346389&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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