# L-Proline, N-(4-chlorobenzoyl)-, octyl ester

**Inchi:** InChI=1S/C20H28ClNO3/c1-2-3-4-5-6-7-15-25-20(24)18-9-8-14-22(18)19(23)16-10-12-1
**InchiKey:** JAAOVWZYOAPJSL-UHFFFAOYSA-N
**Formula:** C20H28ClNO3
**SMILES:** CCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(Cl)cc1
**Mol. weight [g/mol]:** 365.89

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.77 | | Crippen Method |
| logp | 4.848 | | Crippen Method |
| mcvol | 289.270 | ml/mol | McGowan Method |
| rinpol | 2817.00 | | NIST Webbook |
| rinpol | 2817.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U346150&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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