# L-Proline, N-(3-methoxybenzoyl)-, propyl ester

**Inchi:** InChI=1S/C16H21NO4/c1-3-10-21-16(19)14-8-5-9-17(14)15(18)12-6-4-7-13(11-12)20-2/l
**InchiKey:** LBEGTUJQJCRKPN-UHFFFAOYSA-N
**Formula:** C16H21NO4
**SMILES:** CCCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
**Mol. weight [g/mol]:** 291.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.12 | | Crippen Method |
| logp | 2.253 | | Crippen Method |
| mcvol | 226.540 | ml/mol | McGowan Method |
| rinpol | 2376.00 | | NIST Webbook |
| rinpol | 2376.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U346167&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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