# L-Proline, N-(2-chlorobenzoyl)-, methyl ester

**Inchi:** InChI=1S/C13H14ClNO3/c1-18-13(17)11-6-3-7-15(11)12(16)9-4-2-5-10(14)8-9/h2,4-5,8,1
**InchiKey:** GAJYHLOGZCPBPV-UHFFFAOYSA-N
**Formula:** C13H14ClNO3
**SMILES:** COC(=O)C1CCCN1C(=O)c1cccc(Cl)c1
**Mol. weight [g/mol]:** 267.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.84 | | Crippen Method |
| logp | 2.118 | | Crippen Method |
| mcvol | 190.640 | ml/mol | McGowan Method |
| rinpol | 2015.00 | | NIST Webbook |
| rinpol | 2015.00 | | NIST Webbook |

## Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U299589&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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