

# Ipanguline D5

**Inchi:** InChI=1S/C15H25NO6/c1-9(22-10(2)17)15(3,20)14(19)21-8-11-4-6-16-7-5-12(18)13(11)  
**InchiKey:** NWXBPCGWPSVFTO-CVARFHGKSA-N  
**Formula:** C15H25NO6  
**SMILES:** CC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12  
**Mol. weight [g/mol]:** 315.36

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -0.92   |        | Crippen Method |
| logp          | -0.313  |        | Crippen Method |
| mcvol         | 237.090 | ml/mol | McGowan Method |
| rinpol        | 2157.00 |        | NIST Webbook   |
| rinpol        | 2157.00 |        | NIST Webbook   |
| rinpol        | 2157.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395032&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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