# Ipanguline D10

**Inchi:** InChI=1S/C18H31NO6/c1-5-11(2)16(21)25-12(3)18(4,23)17(22)24-10-13-6-8-19-9-7-14(
**InchiKey:** QGMFKSHYVNTQIZ-FCQBRQFGSA-N
**Formula:** C18H31NO6
**SMILES:** CCC(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
**Mol. weight [g/mol]:** 357.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.93 | | Crippen Method |
| logp | 0.714 | | Crippen Method |
| mcvol | 279.360 | ml/mol | McGowan Method |
| rinpol | 2349.00 | | NIST Webbook |
| rinpol | 2327.00 | | NIST Webbook |
| rinpol | 2327.00 | | 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=R394955&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