# Isoipanguline D3

**Inchi:** InChI=1S/C13H23NO5/c1-8(15)13(2,18)12(17)19-7-9-3-5-14-6-4-10(16)11(9)14/h8-11,15
**InchiKey:** GWTMMYYKPSYPDW-UPEKLYLESA-N
**Formula:** C13H23NO5
**SMILES:** CC(O)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
**Mol. weight [g/mol]:** 273.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -0.48 | | Crippen Method |
| logp | -0.883 | | Crippen Method |
| mcvol | 207.340 | ml/mol | McGowan Method |
| rinpol | 2022.00 | | NIST Webbook |
| rinpol | 2022.00 | | 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=R395210&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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