

# Ipanguline 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-LFEBVRLFSA-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	2037.00		NIST Webbook
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rinpol	2037.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R395012&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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