

# Ipanguline C5

**Inchi:** InChI=1S/C23H35NO7/c1-7-14(3)20(25)30-16(5)23(6,28)22(27)29-13-17-9-11-24-12-10-  
**InchiKey:** VSDNNRUBRVNXFZ-XIKQIGSHSA-N  
**Formula:** C23H35NO7  
**SMILES:** CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C(C)(O)C(C)OC(=O)C(C)=CC)C12  
**Mol. weight [g/mol]:** 437.53

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.151		Crippen Method
mcvol	342.780	ml/mol	McGowan Method
rinpol	2645.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R414207&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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