

# Ipanguline B3

**Inchi:** InChI=1S/C24H31NO9/c1-14(32-15(2)26)24(4,34-16(3)27)23(30)31-13-17-9-11-25-12-10  
**InchiKey:** KIUVAQHBLGEXAX-QWOUTQQKSA-N  
**Formula:** C24H31NO9  
**SMILES:** CC(=O)OC(C)C(C)(OC(C)=O)C(=O)OCC1CCN2CCC(OC(=O)c3ccccc3O)C12  
**Mol. weight [g/mol]:** 477.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	1.828		Crippen Method
mcvol	349.150	ml/mol	McGowan Method
rinpol	2927.00		NIST Webbook
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rinpol	2927.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R394891&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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