

# Ipanguline B3

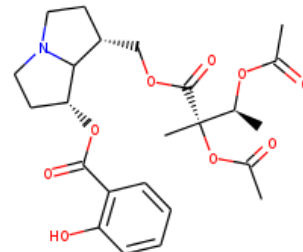
**InChI:** InChI=1S/C24H31NO9/c1-14(32-15(2)26)24(4,34-16(3)27)23(30)31-13-17-9-11-25-12-10-20(21(17)25)33-22(29)18-7-5-6-8-19(18)28/h5-8,14,17,20-21,28H,9-13H2,1-4H3/t14-,17+,20+,21?,24-/m1/s1

**InChI Key:** KIUVAQHBLGEXAX-QWOUTQQKSA-N

**Formula:** C24H31NO9

**SMILES:** CC(=O)OC(C)C(C)(OC(C)=O)C(=O)OCC1CCN2CCC(OC(=O)c3ccccc3O)C12

**Molecular Weight:** 477.50



## Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.83		Crippen Method

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H31NO9/c1-14\(32-15\(2\)26\)24\(4,34-16\(3\)27\)23\(30\)31-13-17-9-11-25-12-10-20\(21\(17\)25\)33-22\(29\)18-7-5-6-8-19\(18\)28/h5-8,14,17,20-21,28H,9-13H2,1-4H3/t14-,17+,20+,21?,24-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H31NO9/c1-14(32-15(2)26)24(4,34-16(3)27)23(30)31-13-17-9-11-25-12-10-20(21(17)25)33-22(29)18-7-5-6-8-19(18)28/h5-8,14,17,20-21,28H,9-13H2,1-4H3/t14-,17+,20+,21?,24-/m1/s1)

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

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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