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: 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices