Ipanguline A4

Inchi: InChI=1S/C26H37NO7/c1-5-17(2)24(29)33-18(3)26(4,31)25(30)32-16-20-11-13-27-14-12
InchiKey: WZILNEZKTCHCAY-NATNDXTASA-N
Formula: C26H37NO7
SMILES: CCC(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)Cc3ccccc3)C12
Mol. weight [g/mol]: 475.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	2.507		Crippen Method
mcvol	369.890	ml/mol	McGowan Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394866&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices