Isoipanguline B2

Inchi: InChI=1S/C22H29NO8/c1-13(30-14(2)24)22(3,28)21(27)29-12-15-8-10-23-11-9-18(19(15
InchiKey: GCEGBPGJRGEBFU-JOPYFQBDSA-N
Formula: C22H29NO8
SMILES: CC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)c3ccccc3O)C12
Mol. weight [g/mol]: 435.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.258		Crippen Method
mcvol	319.400	ml/mol	McGowan Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395181&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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