

Ipanguline 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)20)16-7-6-5-3-2
InchiKey: GCEGBPGJRGEBFU-QWJIFQQTSA-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	2873.00		NIST Webbook
rinpol	2873.00		NIST Webbook
rinpol	2873.00		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=R394886&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

Latest version available from:
<https://www.chemeo.com/cid/34-971-6/lpanguline-B2.pdf>

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