Ipanguline A1

Inchi: InChI=1S/C21H29NO6/c1-14(23)21(2,26)20(25)27-13-16-8-10-22-11-9-17(19(16)22)28-1
InchiKey: ZIZWTEQHLVZFMT-ZOGMDVOISA-N
Formula: C21H29NO6
SMILES: CC(O)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)Cc3ccccc3)C12
Mol. weight [g/mol]: 391.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	0.910		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
rinpol	2707.00		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=R394831&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