Ipanguline C4

Inchi: InChI=1S/C23H39NO7/c1-7-14(3)20(25)30-16(5)23(6,28)22(27)29-13-17-9-11-24-12-10-
InchiKey: AOEBMANFIFKVRE-RVVCJYLJSA-N
Formula: C23H39NO7
SMILES: CCC(C)C(=O)OC1CCN2CCC(COC(=O)C(C)(O)C(C)OC(=O)C(C)CC)C12
Mol. weight [g/mol]: 441.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	2.310		Crippen Method
mcvol	351.380	ml/mol	McGowan Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394935&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