Ipanguline A2

Inchi: InChI=1S/C23H31NO7/c1-15(30-16(2)25)23(3,28)22(27)29-14-18-9-11-24-12-10-19(21(1
InchiKey: RVHJQVQAXBROKU-HAIWMFQASA-N
Formula: C23H31NO7
SMILES: CC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)Cc3ccccc3)C12
Mol. weight [g/mol]: 433.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	1.481		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394846&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.