Ipanguline C1

Inchi: InChI=1S/C18H31NO6/c1-5-11(2)16(21)25-14-7-9-19-8-6-13(15(14)19)10-24-17(22)18(4
InchiKey: GOUCUXKGKNFFFZ-FCQBRQFGSA-N
Formula: C18H31NO6
SMILES: CCC(C)C(=O)OC1CCN2CCC(COC(=O)C(C)(O)C(C)O)C12
Mol. weight [g/mol]: 357.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	0.714		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394900&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