Ipanguline C3

Inchi: InChI=1S/C22H35NO8/c1-7-13(2)20(26)30-18-9-11-23-10-8-17(19(18)23)12-28-21(27)22
InchiKey: ZADUDDBUDFODBU-KIRVMEOHSA-N
Formula: C22H35NO8
SMILES: CCC(C)C(=O)OC1CCN2CCC(COC(=O)C(C)(OC(C)=O)C(C)OC(C)=O)C12
Mol. weight [g/mol]: 441.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.855		Crippen Method
mcvol	338.860	ml/mol	McGowan Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394920&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