Ipanguline A3

Inchi: InChI=1S/C25H33NO8/c1-16(32-17(2)27)25(4,34-18(3)28)24(30)31-15-20-10-12-26-13-1
InchiKey: ZKJDJIORHUYWFV-YHPDBUQDSA-N
Formula: C25H33NO8
SMILES: CC(=O)OC(C)C(C)(OC(C)=O)C(=O)OCC1CCN2CCC(OC(=O)Cc3ccccc3)C12
Mol. weight [g/mol]: 475.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	2.052		Crippen Method
mcvol	357.370	ml/mol	McGowan Method
rinpol	2891.00		NIST Webbook
rinpol	2891.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394851&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

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