Isoipanguline B1

Inchi: InChI=1S/C20H27NO7/c1-12(22)20(2,26)19(25)27-11-13-7-9-21-10-8-16(17(13)21)28-18
InchiKey: HQNBAGWQDKKAMY-HHFZGZQUSA-N
Formula: C20H27NO7
SMILES: CC(O)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)c3ccccc3O)C12
Mol. weight [g/mol]: 393.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	0.687		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395176&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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