

Isoipanguline A1

Inchi: InChI=1S/C21H29NO6/c1-14(23)21(2,26)20(25)27-13-16-8-10-22-11-9-17(19(16)22)28-
InchiKey: ZIZWTEQHLVZFM-ANOOSVGQSA-N
Formula: C21H29NO6
SMILES: CC(O)C(C)(O)C(=O)OCC1CCN2CCC(OC(=O)Cc3ccccc3)C12
Mol. weight [g/mol]: 391.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	0.910		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
rinpol	2702.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395141&Units=SI>

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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<https://www.chemeo.com/cid/65-019-9/Isoipanguline-A1.pdf>

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