Retroisosenine

Inchi: InChI=1S/C18H25NO5/c1-11-8-17(2)9-14(20)23-13-5-7-19-6-4-12(15(13)19)10-22-16(21
InchiKey: KOYQLXLYMDNSGL-HXEPLFAQSA-N
Formula: C18H25NO5
SMILES: CC1CC2(C)CC(=O)OC3CCN4CC=C(COC(=O)C1(C)O2)C34
Mol. weight [g/mol]: 335.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	1.433		Crippen Method
mcvol	247.470	ml/mol	McGowan Method
rinpol	2285.00		NIST Webbook
rinpol	2288.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2283.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178293&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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