Nemorensine-isomer

Inchi: InChI=1S/C18H27NO5/c1-11-8-17(2)9-14(20)23-13-5-7-19-6-4-12(15(13)19)10-22-16(21
InchiKey: DNEINKNDPRUHLP-FBPIHTPSSA-N
Formula: C18H27NO5
SMILES: CC1CC2(C)CC(=O)OC3CCN4CCC(COC(=O)C1(C)O2)C34
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
logp	1.513		Crippen Method
mcvol	251.770	ml/mol	McGowan Method
rinpol	2320.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2325.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177918&Units=SI

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/63-773-4/Nemorensine-isomer.pdf

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