Bulgarsenine

Inchi: InChI=1S/C18H27NO5/c1-11-8-12(2)18(3,22)17(21)23-10-13-4-6-19-7-5-14(16(13)19)24
InchiKey: KUYRTCOXLIWTED-JKHBZPMHSA-N
Formula: C18H27NO5
SMILES: CC1=CC(=O)OC2CCN3CCC(COC(=O)C(C)(O)C(C)C1)C23
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
logp	1.273		Crippen Method
mcvol	258.330	ml/mol	McGowan Method
rinpol	2350.00		NIST Webbook
rinpol	2357.00		NIST Webbook
rinpol	2353.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178139&Units=SI
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):

Legend

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

Latest version available from:
https://www.chemeo.com/cid/55-198-2/Bulgarsenine.pdf

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