Triangularicine

Inchi: InChI=1S/C18H25NO5/c1-4-12(3)17(21)24-15-7-9-19-8-6-14(16(15)19)11-23-18(22)13(5
InchiKey: GOENJWUGVSLZDQ-ATRKRZNXSA-N
Formula: C18H25NO5
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(=CC)CO)C12
Mol. weight [g/mol]: 335.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.361		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2399.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178317&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/47-272-8/Triangularicine.pdf