

Hastacine

Inchi: InChI=1S/C18H27NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)
InchiKey: BTHCJHQOYFUIMG-WEHGYXCESA-N
Formula: C18H27NO5
SMILES: CC=C1CC(C)C(C)(O)C(=O)OCC2CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	1.273		Crippen Method
mcvol	258.330	ml/mol	McGowan Method
rinpol	2440.00		NIST Webbook
rinpol	2453.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178208&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/63-105-5/Hastacine.pdf>

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