

cineverine

Inchi: InChI=1S/C24H32N2O5/c1-29-21-7-6-15(11-22(21)30-2)24(28)31-18-8-9-25-13-16-10-17
InchiKey: NSCGXCFTTLNOMA-YFHPXGLKSA-N
Formula: C24H32N2O5
SMILES: COc1ccc(C(=O)OC2CCN3CC4CC(CN5C(=O)CCCC45)C3C2)cc1OC
Mol. weight [g/mol]: 428.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	2.724		Crippen Method
mcvol	322.530	ml/mol	McGowan Method
rinpol	3550.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R390295&Units=SI>

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/50-427-2/cineverine.pdf>

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