

trans-13-Cinnamoyloxylupanine

Inchi: InChI=1S/C24H30N2O3/c27-22-11-6-10-21-19-15-18(16-26(21)22)20-9-4-5-14-25(20)24
InchiKey: MFZPBYKYOUMGKA-DHJNTMCZSA-N
Formula: C24H30N2O3
SMILES: O=C(C=Cc1cccc1)OC1C2CC(CN3C(=O)CCCC23)C2CCCCN21
Mol. weight [g/mol]: 394.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.454		Crippen Method
mcvol	306.490	ml/mol	McGowan Method
rinpol	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109198&Units=SI>
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>

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/43-905-9/trans-13-Cinnamoyloxylupanine.pdf>

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