

13-trans-Cinnamoyloxylupanine

Inchi: InChI=1S/C24H30N2O3/c27-23-8-4-7-21-18-13-19(16-26(21)23)22-14-20(11-12-25(22)1
InchiKey: PUFYZCKVLOYPHL-JBJSFTJTSA-N
Formula: C24H30N2O3
SMILES: O=C(C=Cc1ccccc1)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 394.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.107		Crippen Method
mcvol	306.490	ml/mol	McGowan Method
rinpol	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R598617&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

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