

13-Cinnamoyloxymultiflorine

Inchi: InChI=1S/C24H30N2O3/c27-20-8-10-25-16-19-12-18(22(25)13-20)15-26-11-9-21(14-23)
InchiKey: HZQDWTKBYSNSDC-VOTSOKGWSA-N
Formula: C24H30N2O3
SMILES: O=C1CCN2CC3CC(CN4CCC(OC(=O)C=Cc5ccccc5)CC34)C2C1
Mol. weight [g/mol]: 394.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	2.759		Crippen Method
mcvol	306.490	ml/mol	McGowan Method
rinsol	3250.00		NIST Webbook
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Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263915&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
rinsol: Non-polar retention indices

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