

# 13«alpha»-cis-Cinnamoyloxylupanine

<b>Inchi:</b>	InChI=1S/C24H30N2O3/c27-23-8-4-7-22-18-13-19(15-26(22)23)21-11-10-20(16-25(21)1
<b>InchiKey:</b>	DHCKHXMBCUZMDX-TWXXOYHDSA-N
<b>Formula:</b>	C24H30N2O3
<b>SMILES:</b>	O=C(C=Cc1ccccc1)OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3
<b>Mol. weight [g/mol]:</b>	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
rropol	3260.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R263831&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R263831&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rropol:</b>	Non-polar retention indices

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