

# 13-Trans-cinnamoyloxylupanine

<b>Inchi:</b>	InChI=1S/C24H30N2O3/c27-23-8-4-7-21-18-13-19(16-26(21)23)22-14-20(11-12-25(22)1
<b>InchiKey:</b>	PUFYZCKVLOYPHL-KVXFRRANSA-N
<b>Formula:</b>	C24H30N2O3
<b>SMILES:</b>	O=C(C=Cc1cccc1)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
<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
rinpola	3390.00		NIST Webbook

## Sources

<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=R308484&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308484&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>rinpola:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/114-792-6/13-Trans-cinnamoyloxylupanine.pdf>

Generated by Cheméo on 2024-04-29 17:35:27.488301152 +0000 UTC m=+16701376.408878462.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.