

# 3«beta»-Angeloyloxylupanine

<b>Inchi:</b>	InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-17-7-8-18(23)22-12-14-10-15(19(17)22)11-2
<b>InchiKey:</b>	PPUAYTALVXQYQS-AHSMOQIKSA-N
<b>Formula:</b>	C20H30N2O3
<b>SMILES:</b>	CC=C(C)C(=O)OC1CCC(=O)N2CC3CC(CN4CCCCC34)C12
<b>Mol. weight [g/mol]:</b>	346.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.360		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
rinpola	2755.00		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=R264027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R264027&amp;Units=SI</a>
<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>

## 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

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