

# 13«alpha»-Benzoyloxylupanine

<b>Inchi:</b>	InChI=1S/C22H28N2O3/c25-21-8-4-7-20-16-11-17(13-24(20)21)19-10-9-18(14-23(19)12
<b>InchiKey:</b>	YOUPTJYGUDWCEW-YFHPXGLKSA-N
<b>Formula:</b>	C22H28N2O3
<b>SMILES:</b>	O=C(OC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3)c1cccc1
<b>Mol. weight [g/mol]:</b>	368.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.707		Crippen Method
mcvol	282.610	ml/mol	McGowan Method
rinsol	3100.00		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=R263826&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R263826&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>rinsol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/17-632-1/13-alpha-Benzoyloxylupanine.pdf>

Generated by Cheméo on 2024-04-19 18:06:58.09522443 +0000 UTC m=+15839267.015801745.

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