

# 3'-benzoylindicine

<b>Inchi:</b>	InChI=1S/C22H29NO6/c1-14(2)22(27,15(3)29-20(25)16-7-5-4-6-8-16)21(26)28-13-17-9-
<b>InchiKey:</b>	QRFQYTMJHJMQOP-KRDZULTMSA-N
<b>Formula:</b>	C22H29NO6
<b>SMILES:</b>	CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)OC(=O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	403.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	1.537		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
rinpol	2727.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R516482&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R516482&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>
<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>

## 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>rinpol:</b>	Non-polar retention indices

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