

# Minalobine O

<b>Inchi:</b>	InChI=1S/C18H29NO5/c1-5-12(2)16(20)24-13(3)18(4,22)17(21)23-11-14-8-10-19-9-6-7-
<b>InchiKey:</b>	QWLVLKBPONBFQZ-LABHKYKLSA-N
<b>Formula:</b>	C18H29NO5
<b>SMILES:</b>	CC=C(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCCC12
<b>Mol. weight [g/mol]:</b>	339.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	1.663		Crippen Method
mcvol	269.190	ml/mol	McGowan Method
rinpola	2236.00		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=R414405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R414405&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/54-005-6/Minalobine-O.pdf>

Generated by Cheméo on 2024-04-20 13:38:18.140099642 +0000 UTC m=+15909547.060676954.

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