

# Amitriptyline M (HO-N-oxide)

<b>Other names:</b>	Amitriptyline N-oxide M(HO)
<b>Inchi:</b>	InChI=1S/C20H23NO2/c1-21(2,23)13-5-8-20-18-7-4-3-6-15(18)9-10-16-14-17(22)11-12-
<b>InchiKey:</b>	BAGNQXUZEMNEPB-ZBKNUEDVSA-N
<b>Formula:</b>	C20H23NO2
<b>SMILES:</b>	<chem>C[N+](C)([O-])CCC=C1c2ccccc2CCc2cc(O)ccc21</chem>
<b>Mol. weight [g/mol]:</b>	309.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	3.887		Crippen Method
mcvol	251.700	ml/mol	McGowan Method
rinpola	2000.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R212952&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R212952&amp;Units=SI</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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