

# Doxepin M(N-oxide)

**Inchi:** InChI=1S/C19H21NO2/c1-20(2,21)13-7-11-17-16-9-4-3-8-15(16)14-22-19-12-6-5-10-18(20)/1  
**InchiKey:** QJCSDPQQGVJGQY-BOPFTXTBSA-N  
**Formula:** C<sub>19</sub>H<sub>21</sub>NO<sub>2</sub>  
**SMILES:** C[N+](C)([O-])CCC=C1c2ccccc2COc2ccccc21  
**Mol. weight [g/mol]:** 295.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.975		Crippen Method
mcvol	237.610	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R213168&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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