

# Trachelanthamidine, 1,2«beta»-epoxy-

<b>Other names:</b>	Supinidine, 1«beta»,2«beta»-epoxy- 1«beta»H-Isoretronecanol, 1,2«beta»-epoxy- 1«beta»,2«beta»-Epoxy-1«alpha»-hydroxymethyl-8«alpha»-pyrrolizidine
<b>Inchi:</b>	InChI=1S/C8H13NO2/c10-5-8-6-2-1-3-9(6)4-7(8)11-8/h6-7,10H,1-5H2
<b>InchiKey:</b>	FRPJEHRSJNAWEI-UHFFFAOYSA-N
<b>Formula:</b>	C8H13NO2
<b>SMILES:</b>	OCC12OC1CN1CCCC12
<b>Mol. weight [g/mol]:</b>	155.19
<b>CAS:</b>	15211-03-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	-0.406		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
rropol	1342.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15211037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15211037&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>rropol:</b>	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/60-640-4/Trachelanthamidine-1-2-beta-epoxy.pdf>

Generated by Cheméo on 2024-04-26 10:13:47.838536988 +0000 UTC m=+16415676.759114300.

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