

# Nalmefene

<b>Other names:</b>	Morphinan-3,14-diol, 17-(cyclopropylmethyl)-4,5-epoxy-6-methylene-, (5«alpha»)-17-(Cyclopropylmethyl)-4,5«alpha»-epoxy-6-methylenemorphinan-3,14-diol Nalmetrene JF-1 ORF-11676
<b>Inchi:</b>	InChI=1S/C21H25NO3/c1-12-6-7-21(24)16-10-14-4-5-15(23)18-17(14)20(21,19(12)25-18
<b>InchiKey:</b>	WJBLNOPPDWQMCH-UHFFFAOYSA-N
<b>Formula:</b>	C21H25NO3
<b>SMILES:</b>	<chem>C=C1CCC2(O)C3Cc4ccc(O)c5c4C2(CCN3CC2CC2)C1O5</chem>
<b>Mol. weight [g/mol]:</b>	339.43
<b>CAS:</b>	55096-26-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	2.512		Crippen Method
mcvol	251.980	ml/mol	McGowan Method
rinpol	2797.60		NIST Webbook
rinpol	2797.60		NIST Webbook

## Sources

<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=C55096269&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55096269&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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