

# Retronecine

<b>Other names:</b>	Relronecine (7R) Retronecine (7R)
<b>Inchi:</b>	InChI=1S/C8H13NO2/c10-5-6-1-3-9-4-2-7(11)8(6)9/h1,7-8,10-11H,2-5H2/t7-,8?/m0/s1
<b>InchiKey:</b>	HJSJELVDQOXCHO-JAMMHFISA-N
<b>Formula:</b>	C8H13NO2
<b>SMILES:</b>	OCC1=CCN2CCC(O)C12
<b>Mol. weight [g/mol]:</b>	155.19
<b>CAS:</b>	480-85-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.14		Crippen Method
logp	-0.646		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1465.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C480853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C480853&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>
<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

**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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