

# 9-Senecioldretronecine

**Inchi:** InChI=1S/C13H19NO3/c1-9(2)7-12(16)17-8-10-3-5-14-6-4-11(15)13(10)14/h3,7,11,13,15  
**InchiKey:** ILQKJOOZWZFSMTN-AAEUAGOB-SA-N  
**Formula:** C13H19NO3  
**SMILES:** CC(C)=CC(=O)OCC1=CCN2CCC(O)C12  
**Mol. weight [g/mol]:** 237.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1833.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R495246&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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