

# 7-Seneciroylheliotridine

**Inchi:** InChI=1S/C13H19NO3/c1-9(2)7-12(16)17-11-4-6-14-5-3-10(8-15)13(11)14/h3,7,11,13,15  
**InchiKey:** JWVMHVYNWULPCC-YPMHNXCESA-N  
**Formula:** C13H19NO3  
**SMILES:** CC(C)=CC(=O)OC1CCN2CC=C(CO)C12  
**Mol. weight [g/mol]:** 237.29  
**CAS:** 146450-65-9

## 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	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1915.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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=C146450659&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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