

# Citronellic acid, picolinyl ester

**Inchi:** InChI=1S/C16H23NO2/c1-13(2)6-4-7-14(3)10-16(18)19-12-15-8-5-9-17-11-15/h5-6,8-9,1  
**InchiKey:** HUYVLPFCDFDEJM-UHFFFAOYSA-N  
**Formula:** C16H23NO2  
**SMILES:** CC(C)=CCCC(C)CC(=O)OCc1cccnc1  
**Mol. weight [g/mol]:** 261.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.897		Crippen Method
mcvol	225.660	ml/mol	McGowan Method
rinpol	1987.90		NIST Webbook
rinpol	1987.90		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=U333629&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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