

(R)-(+)-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	1986.10		NIST Webbook
rinpol	1986.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	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=U333591&Units=SI

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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<https://www.chemeo.com/cid/119-862-3/R-Citronellic-acid-picolinyl-ester.pdf>

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