(S)-(-)-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	1990.30		NIST Webbook
rinpol	1990.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U333553&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.