

10-Undecenoic acid, picolinyl ester

Inchi: InChI=1S/C17H25NO2/c1-2-3-4-5-6-7-8-9-12-17(19)20-15-16-11-10-13-18-14-16/h2,10-
InchiKey: BGLYRRAMMMXUMK-UHFFFAOYSA-N
Formula: C17H25NO2
SMILES: C=CCCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 275.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	4.432		Crippen Method
mcvol	239.750	ml/mol	McGowan Method
rinpole	2155.50		NIST Webbook
rinpole	2155.50		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333570&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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