10-Undecynoic acid, picolinyl ester

Inchi: InChI=1S/C17H23NO2/c1-2-3-4-5-6-7-8-9-12-17(19)20-15-16-11-10-13-18-14-16/h1,10-1
InchiKey: LLCCNDJNRFGKPE-UHFFFAOYSA-N
Formula: C17H23NO2
SMILES: C#CCCCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	3.879		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
rinpol	2188.20		NIST Webbook
rinpol	2188.20		NIST Webbook

Sources

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=U333575&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

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