

9-Decenoic acid, picolinyl ester

Inchi: InChI=1S/C16H23NO2/c1-2-3-4-5-6-7-8-11-16(18)19-14-15-10-9-12-17-13-15/h2,9-10,12-13,15-16,18-19
InchiKey: MVGGDGNWWSKKBD-UHFFFAOYSA-N
Formula: C16H23NO2
SMILES: C=CCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 261.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	4.042		Crippen Method
mcvol	225.660	ml/mol	McGowan Method
rinpol	2054.10		NIST Webbook
rinpol	2054.10		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=U333580&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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