cis-9-Hexadecenoic acid, picolinyl ester

Inchi: InChI=1S/C22H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-22(24)25-20-21-16-15-18-
InchiKey: YLZJHGBUCVQYIZ-FPLPWBNLSA-N
Formula: C22H35NO2
SMILES: CCCCCCC=CCCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 345.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.53		Crippen Method
logp	6.382		Crippen Method
mcvol	310.200	ml/mol	McGowan Method
rinpol	2668.40		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=U333196&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