cis-9, cis-12-Octadecadienoic acid, picolinyl ester

Inchi: InChI=1S/C24H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-24(26)27-22-23-18-

InchiKey: CBIJRFCIJWDVAB-HZJYTTRNSA-N

Formula: C24H37NO2

SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCc1cccnc1

Mol. weight [g/mol]: 371.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	6.938		Crippen Method
mcvol	334.080	ml/mol	McGowan Method
rinpol	2864.00		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=U333208&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