cis-13,16-Docasadienoic acid, picolinyl ester

Inchi: InChI=1S/C28H45NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-28(30)
InchiKey: TYHOZHCQWYUKMK-HZJYTTRNSA-N
Formula: C28H45NO2
SMILES: CCCCCC=CCC=CCCCCCCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.90		Crippen Method
logp	8.499		Crippen Method
mcvol	390.440	ml/mol	McGowan Method
rinpol	3261.80		NIST Webbook
rinpol	3261.80		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333606&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.