cis-8,11,14-Eicosatrienoic acid, picolinyl ester

Inchi: InChI=1S/C26H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-26(28)29-24-
InchiKey: WZUMSGOOPUTINM-QNEBEIHSSA-N
Formula: C26H39NO2
SMILES: CCCCCC=CCC=CCC=CCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.91		Crippen Method
logp	7.494		Crippen Method
mcvol	357.960	ml/mol	McGowan Method
rinpol	3022.50		NIST Webbook
rinpol	3022.50		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333612&Units=SI
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

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.