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

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