

cis-5,8,11,14,17-Eicosapentaenoic acid, picolinyl ester

Inchi:	InChI=1S/C26H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-26(28)29-24-
InchiKey:	ZGIIDDNKYLSQBH-JLNKQSITSA-N
Formula:	C26H35NO2
SMILES:	CCC=CCC=CCC=CCC=CCC=CCCCC(=O)OCc1ccnc1
Mol. weight [g/mol]:	393.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.62		Crippen Method
logp	7.046		Crippen Method
mcvol	349.360	ml/mol	McGowan Method
rmpol	3132.10		NIST Webbook
rmpol	3132.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U333530&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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