

trans-9-Octadecenoic acid, picolinyl ester

Inchi:	InChI=1S/C24H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-24(26)27-22-23-18-
InchiKey:	FBPJZADLPOSZEO-MDZDMXLPSA-N
Formula:	C24H39NO2
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]:	373.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	7.162		Crippen Method
mcvol	338.380	ml/mol	McGowan Method
rinpola	2866.10		NIST Webbook

Sources

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=U333224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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