

«gamma»-Linolenic acid, picolinyl ester

Other names:	(Z,Z,Z)-6,9,12-Octadecatrienoic acid, picolinyl ester
Inchi:	InChI=1S/C24H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-24(26)27-22-23-18-
InchiKey:	GQFLNXHHBUQWAP-QNEBEIHSSA-N
Formula:	C24H35NO2
SMILES:	CCCCC=CCC=CCC=CCCCC(=O)OCc1ccncc1
Mol. weight [g/mol]:	369.54
CAS:	103418-44-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.07		Crippen Method
logp	6.714		Crippen Method
mcvol	329.780	ml/mol	McGowan Method
rinpol	2842.50		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103418446&Units=SI

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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