

# cis, cis, cis-9, 12, 15-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:	VMDODSILOLPSBY-PDBXOOCHSA-N
Formula:	C24H35NO2
SMILES:	CCC=CCC=CCC=CCCCCCCC(=O)OCc1cccnc1
Mol. weight [g/mol]:	369.54

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.07		Crippen Method
logp	6.714		Crippen Method
mcvol	329.780	ml/mol	McGowan Method
rmpol	2871.20		NIST Webbook
rmpol	2871.20		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333202&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333202&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## 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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