

# 2,6-Pyridinedicarboxylic acid, 1-methoxydec-4-yl nonyl ester

<b>Inchi:</b>	InChI=1S/C27H45NO5/c1-4-6-8-10-11-12-14-22-32-26(29)24-19-15-20-25(28-24)27(30)
<b>InchiKey:</b>	CLSHJIFOIHVGEY-UHFFFAOYSA-N
<b>Formula:</b>	C27H45NO5
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCCCC)CCOC)n1
<b>Mol. weight [g/mol]:</b>	463.65

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	6.911		Crippen Method
mcvol	398.260	ml/mol	McGowan Method
rinsol	3087.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369250&amp;Units=SI</a>

## Legend

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

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