

# 2,6-Pyridinedicarboxylic acid, nonyl 4-octyl ester

Inchi:	InChI=1S/C24H39NO4/c1-4-7-9-10-11-12-13-19-28-23(26)21-17-14-18-22(25-21)24(27)2
InchiKey:	VCFJACLJTIFPKM-UHFFFAOYSA-N
Formula:	C24H39NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)n1
Mol. weight [g/mol]:	405.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.11		Crippen Method
logp	6.505		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
rinpola	2765.00		NIST Webbook
rinpola	2765.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U368838&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368838&amp;Units=SI</a>

## 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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