

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

<b>Inchi:</b>	InChI=1S/C22H26ClNO4/c1-2-3-4-5-6-7-15-27-21(25)19-9-8-10-20(24-19)22(26)28-16-1
<b>InchiKey:</b>	VVYAAJCIRUSJGI-UHFFFAOYSA-N
<b>Formula:</b>	C22H26ClNO4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
<b>Mol. weight [g/mol]:</b>	403.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	5.609		Crippen Method
mcvol	310.420	ml/mol	McGowan Method
rinpola	3051.00		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=U369143&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369143&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>rinpola:</b>	Non-polar retention indices

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