

# 2,6-Pyridinedicarboxylic acid, hexyl 2-isopropoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C22H27NO5/c1-4-5-6-9-15-26-21(24)17-11-10-12-18(23-17)22(25)28-20-14-8
<b>InchiKey:</b>	MXWKOSJPINXSHB-UHFFFAOYSA-N
<b>Formula:</b>	C22H27NO5
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1
<b>Mol. weight [g/mol]:</b>	385.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	4.825		Crippen Method
mcvol	304.050	ml/mol	McGowan Method
rinsol	2793.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369127&amp;Units=SI</a>
<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>

## 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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