

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

<b>Inchi:</b>	InChI=1S/C23H37NO4/c1-4-6-8-10-11-13-18-27-22(25)20-16-14-17-21(24-20)23(26)28-
<b>InchiKey:</b>	BFLORCCZUOGEKM-UHFFFAOYSA-N
<b>Formula:</b>	C23H37NO4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCCC)n1
<b>Mol. weight [g/mol]:</b>	391.54

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69		Crippen Method
logp	6.115		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpola	2718.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U368304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368304&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>rinpola:</b>	Non-polar retention indices

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