

# 2,6-Pyridinedicarboxylic acid, butyl 2-pentyl ester

<b>Inchi:</b>	InChI=1S/C16H23NO4/c1-4-6-11-20-15(18)13-9-7-10-14(17-13)16(19)21-12(3)8-5-2/h7,9
<b>InchiKey:</b>	KUMCOZZQVMIKIF-UHFFFAOYSA-N
<b>Formula:</b>	C16H23NO4
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)OC(C)CCC)n1
<b>Mol. weight [g/mol]:</b>	293.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.384		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpola	2010.00		NIST Webbook

## Sources

<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=U368333&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368333&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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