

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

<b>Inchi:</b>	InChI=1S/C17H25NO4/c1-4-6-11-21-16(19)14-9-7-10-15(18-14)17(20)22-12-13(3)8-5-2/
<b>InchiKey:</b>	PMZMKDPPYLOAAK-UHFFFAOYSA-N
<b>Formula:</b>	C17H25NO4
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)OCC(C)CCC)n1
<b>Mol. weight [g/mol]:</b>	307.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.632		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpola	2202.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369083&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369083&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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