

# 2,6-Pyridinedicarboxylic acid, isobutyl isopropyl ester

<b>Inchi:</b>	InChI=1S/C14H19NO4/c1-9(2)8-18-13(16)11-6-5-7-12(15-11)14(17)19-10(3)4/h5-7,9-10
<b>InchiKey:</b>	ZOUBBDRNLQGAHW-UHFFFAOYSA-N
<b>Formula:</b>	C14H19NO4
<b>SMILES:</b>	CC(C)COC(=O)c1cccc(C(=O)OC(C)C)n1
<b>Mol. weight [g/mol]:</b>	265.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	2.460		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinpola	1841.00		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=U369147&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369147&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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