

# 2,6-Pyridinedicarboxylic acid, isobutyl 2-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C18H19NO5/c1-12(2)11-23-17(20)13-7-6-8-14(19-13)18(21)24-16-10-5-4-9-15
<b>InchiKey:</b>	YOYREAMWLOS NHB-UHFFFAOYSA-N
<b>Formula:</b>	C18H19NO5
<b>SMILES:</b>	COc1ccccc1OC(=O)c1cccc(C(=O)OCC(C)C)n1
<b>Mol. weight [g/mol]:</b>	329.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.122		Crippen Method
mcvol	247.690	ml/mol	McGowan Method
rinpol	2527.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369215&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369215&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/14-423-6/2-6-Pyridinedicarboxylic-acid-isobutyl-2-methoxyphenyl-ester.pdf>

Generated by Cheméo on 2024-04-26 20:24:14.768598738 +0000 UTC m=+16452303.689176059.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.