

# 2,6-Pyridinedicarboxylic acid, dodecyl isopropyl ester

<b>Inchi:</b>	InChI=1S/C22H35NO4/c1-4-5-6-7-8-9-10-11-12-13-17-26-21(24)19-15-14-16-20(23-19)2
<b>InchiKey:</b>	AEAJBYJQVUNZFP-UHFFFAOYSA-N
<b>Formula:</b>	C22H35NO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C)n1
<b>Mol. weight [g/mol]:</b>	377.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	5.724		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpola	2689.00		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=U369157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369157&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>rinpola:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/28-966-9/2-6-Pyridinedicarboxylic-acid-dodecyl-isopropyl-ester.pdf>

Generated by Cheméo on 2024-04-23 16:05:21.264987175 +0000 UTC m=+16177570.185564490.

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