

# 2,6-Pyridinedicarboxylic acid, 2-isopropoxyphenyl nonyl ester

**Inchi:** InChI=1S/C25H33NO5/c1-4-5-6-7-8-9-12-18-29-24(27)20-14-13-15-21(26-20)25(28)31-2  
**InchiKey:** NGUFINCNUIQCFP-UHFFFAOYSA-N  
**Formula:** C25H33NO5  
**SMILES:** CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1  
**Mol. weight [g/mol]:** 427.53

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.98		Crippen Method
logp	5.995		Crippen Method
mcvol	346.320	ml/mol	McGowan Method
rinpola	3045.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369129&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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