

# 2,6-Pyridinedicarboxylic acid, nonyl phenethyl ester

**Inchi:** InChI=1S/C24H31NO4/c1-2-3-4-5-6-7-11-18-28-23(26)21-15-12-16-22(25-21)24(27)29-1  
**InchiKey:** TZXMEIHXLPLWEM-UHFFFAOYSA-N  
**Formula:** C24H31NO4  
**SMILES:** CCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1  
**Mol. weight [g/mol]:** 397.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.389		Crippen Method
mcvol	326.360	ml/mol	McGowan Method
rinsol	3044.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369229&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/26-331-5/2-6-Pyridinedicarboxylic-acid-nonyl-phenethyl-ester.pdf>

Generated by Cheméo on 2024-05-03 00:03:49.604590204 +0000 UTC m=+16983878.525167519.

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