

# 2,6-Pyridinedicarboxylic acid, octyl 2,4,4-trimethylpentyl ester

**Inchi:** InChI=1S/C23H37NO4/c1-6-7-8-9-10-11-15-27-21(25)19-13-12-14-20(24-19)22(26)28-17  
**InchiKey:** LGQJZJZBUWRWNP-UHFFFAOYSA-N  
**Formula:** C23H37NO4  
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1  
**Mol. weight [g/mol]:** 391.54

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.828		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinsol	2665.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368794&Units=SI>  
**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)

## 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/34-249-8/2-6-Pyridinedicarboxylic-acid-octyl-2-4-4-trimethylpentyl-ester.pdf>

Generated by Cheméo on 2024-04-18 23:35:54.46473857 +0000 UTC m=+15772603.385315887.

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