

# 2,6-Pyridinedicarboxylic acid, 3-methylbutyl undecyl ester

**Inchi:** InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-17-27-22(25)20-14-13-15-21(24-20)23(2  
**InchiKey:** BWUQYCJPBKOVMR-UHFFFAOYSA-N  
**Formula:** C23H37NO4  
**SMILES:** CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1  
**Mol. weight [g/mol]:** 391.54

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	5.972		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpola	2808.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368323&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  
**rinpola:** Non-polar retention indices

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