

# 2,6-Pyridinedicarboxylic acid, dodecyl 2-methylbutyl ester

**Inchi:** InChI=1S/C24H39NO4/c1-4-6-7-8-9-10-11-12-13-14-18-28-23(26)21-16-15-17-22(25-21)  
**InchiKey:** ATPWDCVSRMHMJ-UHFFFAOYSA-N  
**Formula:** C24H39NO4  
**SMILES:** CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)n1  
**Mol. weight [g/mol]:** 405.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	6.362		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369068&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## Legend

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

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