

# 2,6-Pyridinedicarboxylic acid, decyl pentyl ester

**Inchi:** InChI=1S/C22H35NO4/c1-3-5-7-8-9-10-11-13-18-27-22(25)20-16-14-15-19(23-20)21(24)  
**InchiKey:** YGMVXJTZZIEQDU-UHFFFAOYSA-N  
**Formula:** C22H35NO4  
**SMILES:** CCCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1  
**Mol. weight [g/mol]:** 377.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	5.726		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpola	2749.00		NIST Webbook
rinpola	2749.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368288&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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