

# 2,6-Pyridinedicarboxylic acid, hexadecyl pentyl ester

**Inchi:** InChI=1S/C28H47NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-24-33-28(31)26-22-20  
**InchiKey:** GQZXHENPPNLZRE-UHFFFAOYSA-N  
**Formula:** C28H47NO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1  
**Mol. weight [g/mol]:** 461.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.68		Crippen Method
logp	8.067		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinpole	3220.00		NIST Webbook
rinpole	3220.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368294&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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  
**rinpole:** Non-polar retention indices

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