

# 2,6-Pyridinedicarboxylic acid, isobutyl pentyl ester

**Inchi:** InChI=1S/C16H23NO4/c1-4-5-6-10-20-15(18)13-8-7-9-14(17-13)16(19)21-11-12(2)3/h7-9  
**InchiKey:** YPRIGABXAUBAAN-UHFFFAOYSA-N  
**Formula:** C16H23NO4  
**SMILES:** CCCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1  
**Mol. weight [g/mol]:** 293.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.241		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpola	2111.00		NIST Webbook
rinpola	2111.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368281&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)  
**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  
**rinpola:** Non-polar retention indices

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