

# 2,6-Pyridinedicarboxylic acid, di(2-methylbutyl) ester

**Inchi:** InChI=1S/C17H25NO4/c1-5-12(3)10-21-16(19)14-8-7-9-15(18-14)17(20)22-11-13(4)6-2/1  
**InchiKey:** QXPNMURBGYIKDZ-UHFFFAOYSA-N  
**Formula:** C17H25NO4  
**SMILES:** CCC(C)COC(=O)c1cccc(C(=O)OCC(C)CC)n1  
**Mol. weight [g/mol]:** 307.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.487		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpole	2179.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369073&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  
**rinpole:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/48-463-5/2-6-Pyridinedicarboxylic-acid-di-2-methylbutyl-ester.pdf>

Generated by Cheméo on 2024-04-26 08:53:42.664846936 +0000 UTC m=+16410871.585424252.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.