

# 2,6-Pyridinedicarboxylic acid, ethyl 2-ethylhexyl ester

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

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.632		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpole	2192.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368265&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

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