

# 2,6-Pyridinedicarboxylic acid, 2-methylhex-3-yl 2-octyl ester

**Inchi:** InChI=1S/C22H35NO4/c1-6-8-9-10-13-17(5)26-21(24)18-14-11-15-19(23-18)22(25)27-20  
**InchiKey:** HVMDNYJDJNUIHP-UHFFFAOYSA-N  
**Formula:** C22H35NO4  
**SMILES:** CCCCCC(C)OC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1  
**Mol. weight [g/mol]:** 377.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	5.579		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpola	2437.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368301&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  
**rinpola:** Non-polar retention indices

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