

# 2,6-Pyridinedicarboxylic acid, 2-ethylbutyl hexadecyl ester

**Inchi:** InChI=1S/C29H49NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-33-28(31)26-21-20  
**InchiKey:** DMSQBHWHCBNOLA-UHFFFAOYSA-N  
**Formula:** C<sub>29</sub>H<sub>49</sub>NO<sub>4</sub>  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(CC)CC)n1  
**Mol. weight [g/mol]:** 475.70

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.85		Crippen Method
logp	8.313		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3247.00		NIST Webbook
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## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369052&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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