

# 2,6-Pyridinedicarboxylic acid, hexadecyl 4-octyl ester

**Inchi:** InChI=1S/C31H53NO4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-26-35-30(33)28-24-2  
**InchiKey:** HHSOXFQRXGHEHM-UHFFFAOYSA-N  
**Formula:** C31H53NO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)n1  
**Mol. weight [g/mol]:** 503.76

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -11.04  |        | Crippen Method |
| logp          | 9.235   |        | Crippen Method |
| mcvol         | 448.750 | ml/mol | McGowan Method |
| rinpol        | 3291.00 |        | NIST Webbook   |
| rinpol        | 3291.00 |        | NIST Webbook   |

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368845&Units=SI>

## 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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