

# 2,6-Pyridinedicarboxylic acid, butyl pentadecyl ester

**Inchi:** InChI=1S/C26H43NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-22-31-26(29)24-20-18-19  
**InchiKey:** LKFIYCXPSTQKST-UHFFFAOYSA-N  
**Formula:** C<sub>26</sub>H<sub>43</sub>NO<sub>4</sub>  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1  
**Mol. weight [g/mol]:** 433.62

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -8.84   |        | Crippen Method |
| logp          | 7.287   |        | Crippen Method |
| mcvol         | 378.300 | ml/mol | McGowan Method |
| rinpol        | 3104.00 |        | NIST Webbook   |

## 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=U369078&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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