

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

**Inchi:** InChI=1S/C22H35NO4/c1-6-9-12-17(8-3)15-26-21(24)18-13-10-14-19(23-18)22(25)27-20  
**InchiKey:** ZZDRMDAGGNKPPL-UHFFFAOYSA-N  
**Formula:** C22H35NO4  
**SMILES:** CCCCC(CC)COC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1  
**Mol. weight [g/mol]:** 377.52

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.79   |        | Crippen Method |
| logp          | 5.436   |        | Crippen Method |
| mcvol         | 321.940 | ml/mol | McGowan Method |
| rinpol        | 2473.00 |        | NIST Webbook   |
| rinpol        | 2473.00 |        | 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=U368269&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

Latest version available from:

<https://www.chemeo.com/cid/19-345-8/2-6-Pyridinedicarboxylic-acid-2-ethylhexyl-2-methylhex-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-20 14:02:41.984961709 +0000 UTC m=+15911010.905539030.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.