

# 2,6-Pyridinedicarboxylic acid, heptyl phenethyl ester

**Inchi:** InChI=1S/C22H27NO4/c1-2-3-4-5-9-16-26-21(24)19-13-10-14-20(23-19)22(25)27-17-15  
**InchiKey:** ONEBXWZXRYIRIU-UHFFFAOYSA-N  
**Formula:** C22H27NO4  
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1  
**Mol. weight [g/mol]:** 369.45

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.27   |        | Crippen Method |
| logp          | 4.608   |        | Crippen Method |
| mcvol         | 298.180 | ml/mol | McGowan Method |
| rinpola       | 2880.00 |        | NIST Webbook   |

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369227&Units=SI>

## 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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