

# 2,6-Pyridinedicarboxylic acid, isobutyl nonyl ester

**Inchi:** InChI=1S/C20H31NO4/c1-4-5-6-7-8-9-10-14-24-19(22)17-12-11-13-18(21-17)20(23)25-1  
**InchiKey:** IHOKVKLGLWUMEJ-UHFFFAOYSA-N  
**Formula:** C20H31NO4  
**SMILES:** CCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1  
**Mol. weight [g/mol]:** 349.46

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.09   |        | Crippen Method |
| logp          | 4.802   |        | Crippen Method |
| mcvol         | 293.760 | ml/mol | McGowan Method |
| rinpol        | 2503.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368855&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>

## 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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