# 2,6-Pyridinedicarboxylic acid, isobutyl 5-methoxy-3-methylpent-2-yl ester

**Inchi:** InChI=1S/C18H27NO5/c1-12(2)11-23-17(20)15-7-6-8-16(19-15)18(21)24-14(4)13(3)9-10

**InchiKey:** FAYCDAPUOWBJLT-UHFFFAOYSA-N

**Formula:** C18H27NO5

**SMILES:** COCCC(C)C(C)OC(=O)c1cccc(C(=O)OCC(C)C)n1

**Mol. weight [g/mol]:** 337.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.21 | | Crippen Method |
| logp | 3.112 | | Crippen Method |
| mcvol | 271.450 | ml/mol | McGowan Method |
| rinpol | 2291.00 | | NIST Webbook |
| rinpol | 2291.00 | | NIST Webbook |

## Sources

**Crippen Method:** 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=U369172&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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