

# 2,6-Pyridinedicarboxylic acid, isobutyl 2-methylphenyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C18H19NO4/c1-12(2)11-22-17(20)14-8-6-9-15(19-14)18(21)23-16-10-5-4-7-13 |
| <b>InchiKey:</b>            | VPNRKQYCENFJMG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C18H19NO4  |
| <b>SMILES:</b>              | Cc1ccccc1OC(=O)c1cccc(C(=O)OCC(C)C)n1  |
| <b>Mol. weight [g/mol]:</b> | 313.35   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.06   |        | Crippen Method |
| logp          | 3.422   |        | Crippen Method |
| mcvol         | 241.820 | ml/mol | McGowan Method |
| rinsol        | 2391.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369120&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinsol:</b>  | Non-polar retention indices         |

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