

# 2,6-Pyridinedicarboxylic acid, isobutyl phenethyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C19H21NO4/c1-14(2)13-24-19(22)17-10-6-9-16(20-17)18(21)23-12-11-15-7-4 |
| <b>InchiKey:</b>            | TZKVLZPGKZHHNX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C19H21NO4   |
| <b>SMILES:</b>              | CC(C)COC(=O)c1cccc(C(=O)OCCc2ccccc2)n1  |
| <b>Mol. weight [g/mol]:</b> | 327.37  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.77   |        | Crippen Method |
| logp          | 3.294   |        | Crippen Method |
| mcvol         | 255.910 | ml/mol | McGowan Method |
| rinpola       | 2523.00 |        | 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=U369223&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369223&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>rinpola:</b> | Non-polar retention indices         |

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