

2,6-Pyridinedicarboxylic acid, diphenethyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C23H21NO4/c25-22(27-16-14-18-8-3-1-4-9-18)20-12-7-13-21(24-20)23(26)28 |
| InchiKey: | RRGBJJFILZVCBH-UHFFFAOYSA-N |
| Formula: | C23H21NO4 |
| SMILES: | O=C(OCCc1ccccc1)c1cccc(C(=O)OCCc2ccccc2)n1 |
| Mol. weight [g/mol]: | 375.42 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.79 | | Crippen Method |
| logp | 3.881 | | Crippen Method |
| mcvol | 288.510 | ml/mol | McGowan Method |
| rmpol | 3095.00 | | NIST Webbook |
| rmpol | 3095.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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=U369232&Units=SI |

Legend

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

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