

2,6-Pyridinedicarboxylic acid, hexyl isobutyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C17H25NO4/c1-4-5-6-7-11-21-16(19)14-9-8-10-15(18-14)17(20)22-12-13(2)3/ |
| InchiKey: | JWCOERBBUWTZJO-UHFFFAOYSA-N |
| Formula: | C17H25NO4 |
| SMILES: | CCCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1 |
| Mol. weight [g/mol]: | 307.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.83 | | Crippen Method |
| logp | 3.632 | | Crippen Method |
| mcvol | 251.490 | ml/mol | McGowan Method |
| rinpola | 2213.00 | | 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=U368852&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

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