

2,6-Pyridinedicarboxylic acid, heptyl neopentyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C19H29NO4/c1-5-6-7-8-9-13-23-17(21)15-11-10-12-16(20-15)18(22)24-14-19 |
| InchiKey: | DQUBKWQWKZHKTH-UHFFFAOYSA-N |
| Formula: | C19H29NO4 |
| SMILES: | CCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1 |
| Mol. weight [g/mol]: | 335.44 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.67 | | Crippen Method |
| logp | 4.412 | | Crippen Method |
| mcvol | 279.670 | ml/mol | McGowan Method |
| rinpola | 2321.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369003&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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