

# 2,6-Pyridinedicarboxylic acid, hexadecyl neopentyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C28H47NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-32-26(30)24-20-19 |
| <b>InchiKey:</b>            | UHABPVNCTBEHEY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C28H47NO4   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1                                 |
| <b>Mol. weight [g/mol]:</b> | 461.68  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -9.43   |        | Crippen Method |
| logp          | 7.923   |        | Crippen Method |
| mcvol         | 406.480 | ml/mol | McGowan Method |
| rinpola       | 3143.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369012&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369012&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>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                     |

## 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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