

2,6-Pyridinedicarboxylic acid, ethyl hexadecyl ester

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| Inchi: | InChI=1S/C25H41NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-21-30-25(28)23-20-18-1 |
| InchiKey: | TYLYQJMCQPGVOT-UHFFFAOYSA-N |
| Formula: | C25H41NO4 |
| SMILES: | CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC)n1 |
| Mol. weight [g/mol]: | 419.60 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.42 | | Crippen Method |
| logp | 6.896 | | Crippen Method |
| mcvol | 364.210 | ml/mol | McGowan Method |
| rinsol | 3054.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369032&Units=SI |
| 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 |

Legend

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

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