

2,6-Pyridinedicarboxylic acid, dodecyl 3-methylbutyl ester

Inchi: InChI=1S/C24H39NO4/c1-4-5-6-7-8-9-10-11-12-13-18-28-23(26)21-15-14-16-22(25-21)2
InchiKey: HQXBPJMRWAHQBW-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]: 405.57

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.76 | | Crippen Method |
| logp | 6.362 | | Crippen Method |
| mcvol | 350.120 | ml/mol | McGowan Method |
| rinsol | 2906.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U368324&Units=SI>

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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