

# 3,4-Pyridinedicarboxylic acid, dimethyl ester

|                      |                                                                                                               |
|----------------------|---------------------------------------------------------------------------------------------------------------|
| Other names:         | Cinchomeric acid, dimethyl ester<br>Dimethyl 3,4-pyridinedicarboxylate<br>Dimethyl pyridine-3,4-dicarboxylate |
| Inchi:               | InChI=1S/C9H9NO4/c1-13-8(11)6-3-4-10-5-7(6)9(12)14-2/h3-5H,1-2H3                                              |
| InchiKey:            | AUQUSBAFIHOGHK-UHFFFAOYSA-N                                                                                   |
| Formula:             | C9H9NO4                                                                                                       |
| SMILES:              | COC(=O)c1ccncc1C(=O)OC                                                                                        |
| Mol. weight [g/mol]: | 195.17                                                                                                        |
| CAS:                 | 1796-83-4                                                                                                     |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.72   |        | Crippen Method |
| logp          | 0.655   |        | Crippen Method |
| mcvol         | 138.770 | ml/mol | McGowan Method |
| rinpol        | 1502.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1796834&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1796834&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

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

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