

2,6-Pyridinedicarboxylic acid, 2-chlorophenyl ethyl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C15H12ClNO4/c1-2-20-14(18)11-7-5-8-12(17-11)15(19)21-13-9-4-3-6-10(13)1 |
| InchiKey: | FGKISQOJJDYMC5-UHFFFAOYSA-N |
| Formula: | C15H12ClNO4 |
| SMILES: | CCOC(=O)c1cccc(C(=O)Oc2ccccc2Cl)n1 |
| Mol. weight [g/mol]: | 305.71 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.67 | | Crippen Method |
| logp | 3.131 | | Crippen Method |
| mcvol | 211.790 | ml/mol | McGowan Method |
| rinpola | 2376.00 | | 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=U369131&Units=SI |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-126-7/2-6-Pyridinedicarboxylic-acid-2-chlorophenyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-27 18:25:40.767991778 +0000 UTC m=+16531589.688569094.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.