

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

Inchi: InChI=1S/C18H19NO5/c1-4-22-17(20)13-8-7-9-14(19-13)18(21)24-16-11-6-5-10-15(16)2
InchiKey: KUNFQYDMUZUYCF-UHFFFAOYSA-N
Formula: C18H19NO5
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1
Mol. weight [g/mol]: 329.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.05 | | Crippen Method |
| logp | 3.265 | | Crippen Method |
| mcvol | 247.690 | ml/mol | McGowan Method |
| rinpole | 2427.00 | | NIST Webbook |

Sources

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=U369125&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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