2,6-Pyridinedicarboxylic acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C25H25NO6/c1-16(2)29-20-12-5-7-14-22(20)31-24(27)18-10-9-11-19(26-18)25

InchiKey: YDMVMUPRNYSZFF-UHFFFAOYSA-N

Formula: C25H25NO6

SMILES: CC(C)Oc1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1

Mol. weight [g/mol]: 435.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.55		Crippen Method
logp	5.094		Crippen Method
mcvol	328.430	ml/mol	McGowan Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U369130&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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