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

Inchi: InChI=1S/C21H17NO4/c1-14-8-3-5-12-18(14)25-20(23)16-10-7-11-17(22-16)21(24)26-19

InchiKey: ZUGNNOSYWPYXLS-UHFFFAOYSA-N

Formula: C21H17NO4

SMILES: Cc1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2C)n1

Mol. weight [g/mol]: 347.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	4.137		Crippen Method
mcvol	260.330	ml/mol	McGowan Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369124&Units=SI

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

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.