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

Inchi: InChI=1S/C21H17NO6/c1-25-16-10-3-5-12-18(16)27-20(23)14-8-7-9-15(22-14)21(24)28-

InchiKey: UADMVHIJMDNHEN-UHFFFAOYSA-N

Formula: C21H17NO6

SMILES: COc1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2OC)n1

Mol. weight [g/mol]: 379.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	3.537		Crippen Method
mcvol	272.070	ml/mol	McGowan Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		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=U369221&Units=SI

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

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.