2,6-Pyridinedicarboxylic acid, isobutyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H19NO5/c1-12(2)11-23-17(20)13-7-6-8-14(19-13)18(21)24-16-10-5-4-9-15

InchiKey: YOYREAMWLOSNHB-UHFFFAOYSA-N

Formula: C18H19NO5

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

Mol. weight [g/mol]: 329.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.122		Crippen Method
mcvol	247.690	ml/mol	McGowan Method
rinpol	2527.00		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=U369215&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