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

Inchi: InChI=1S/C18H19NO4/c1-12(2)11-22-17(20)14-8-6-9-15(19-14)18(21)23-16-10-5-4-7-13

InchiKey: VPNRKQYCENFJMG-UHFFFAOYSA-N

Formula: C18H19NO4

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

Mol. weight [g/mol]: 313.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	3.422		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
rinpol	2391.00		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=U369120&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

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