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

Inchi: InChI=1S/C17H17NO4/c1-3-11-21-16(19)13-8-6-9-14(18-13)17(20)22-15-10-5-4-7-12(15

InchiKey: UXGSVBUQCUCNEO-UHFFFAOYSA-N

Formula: C17H17NO4

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

Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	3.176		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
rinpol	2352.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369119&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