2,6-Pyridinedicarboxylic acid, diisopropyl ester

Inchi: InChI=1S/C13H17NO4/c1-8(2)17-12(15)10-6-5-7-11(14-10)13(16)18-9(3)4/h5-9H,1-4H3
InchiKey: CPWRDMOUBGOUGY-UHFFFAOYSA-N
Formula: C13H17NO4
SMILES: CC(C)OC(=O)c1cccc(C(=O)OC(C)C)n1
Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.212		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
rinpol	1725.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369164&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices