2,6-Pyridinedicarboxylic acid, isopropyl tridecyl ester

Inchi: InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-14-18-27-22(25)20-16-15-17-21(24-2

InchiKey: BUKDTGBPAWUPGY-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C)n1

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69		Crippen Method
logp	6.115		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2791.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369158&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