2,6-Pyridinedicarboxylic acid, heptyl isobutyl ester

Inchi: InChI=1S/C18H27NO4/c1-4-5-6-7-8-12-22-17(20)15-10-9-11-16(19-15)18(21)23-13-14(2

InchiKey: DVLWEHZNOZOHIW-UHFFFAOYSA-N

Formula: C18H27NO4

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

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.022		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368853&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