2,6-Pyridinedicarboxylic acid, heptyl 2-octyl ester

Inchi: InChI=1S/C22H35NO4/c1-4-6-8-10-12-17-26-21(24)19-15-13-16-20(23-19)22(25)27-18(3

InchiKey: NJWMVLZSKNXCOF-UHFFFAOYSA-N

Formula: C22H35NO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCCCC)n1

Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	5.724		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpol	2628.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368303&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