2,6-Pyridinedicarboxylic acid, heptyl phenethyl ester

Inchi: InChI=1S/C22H27NO4/c1-2-3-4-5-9-16-26-21(24)19-13-10-14-20(23-19)22(25)27-17-15-

InchiKey: ONEBXWZXRYIRIU-UHFFFAOYSA-N

Formula: C22H27NO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1

Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.608		Crippen Method
mcvol	298.180	ml/mol	McGowan Method
rinpol	2880.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369227&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices