2,6-Pyridinedicarboxylic acid, octyl phenethyl ester

Inchi: InChI=1S/C23H29NO4/c1-2-3-4-5-6-10-17-27-22(25)20-14-11-15-21(24-20)23(26)28-18-

InchiKey: YDZUQTIQGBFEJQ-UHFFFAOYSA-N

Formula: C23H29NO4

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

Mol. weight [g/mol]: 383.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	4.998		Crippen Method
mcvol	312.270	ml/mol	McGowan Method
rinpol	2966.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369228&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