2,6-Pyridinedicarboxylic acid, hexyl phenethyl ester

Inchi: InChI=1S/C21H25NO4/c1-2-3-4-8-15-25-20(23)18-12-9-13-19(22-18)21(24)26-16-14-17-

InchiKey: DVCYEAVXFBCDEZ-UHFFFAOYSA-N

Formula: C21H25NO4

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

Mol. weight [g/mol]: 355.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	4.218		Crippen Method
mcvol	284.090	ml/mol	McGowan Method
rinpol	2782.00		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=U369226&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