2,6-Pyridinedicarboxylic acid, di(2-pentyl) ester

Inchi: InChI=1S/C17H25NO4/c1-5-8-12(3)21-16(19)14-10-7-11-15(18-14)17(20)22-13(4)9-6-2/h

InchiKey: YQTJUERRTARQIW-UHFFFAOYSA-N

Formula: C17H25NO4

SMILES: CCCC(C)OC(=O)c1cccc(C(=O)OC(C)CCC)n1

Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	3.772		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2062.00		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=U368349&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