2,6-Pyridinedicarboxylic acid, dipentyl ester

Inchi: InChI=1S/C17H25NO4/c1-3-5-7-12-21-16(19)14-10-9-11-15(18-14)17(20)22-13-8-6-4-2/h
InchiKey: PONGQFFDPLOECH-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.776		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368283&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.