2,6-Pyridinedicarboxylic acid, pentadecyl 2-pentyl ester

Inchi: InChI=1S/C27H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-22-31-26(29)24-20-18-21-

InchiKey: OVGFDVQXPSIASH-UHFFFAOYSA-N

Formula: C27H45NO4

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

Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.37		Crippen Method
logp	7.675		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
rinpol	3101.00		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=U368345&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