2,6-Pyridinedicarboxylic acid, neopentyl nonyl ester

Inchi: InChI=1S/C21H33NO4/c1-5-6-7-8-9-10-11-15-25-19(23)17-13-12-14-18(22-17)20(24)26-

InchiKey: LOHRXFIPFBWNLJ-UHFFFAOYSA-N

Formula: C21H33NO4

SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1

Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	5.192		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinpol	2515.00		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=U369005&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