2,6-Pyridinedicarboxylic acid, neopentyl pentyl ester

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

InchiKey: SDSYBHUXSQWXRP-UHFFFAOYSA-N

Formula: C17H25NO4

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

Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.632		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2128.00		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=U369000&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