2,6-Pyridinedicarboxylic acid, 2-methylhex-3-yl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C22H35NO4/c1-8-10-19(15(2)3)27-21(25)18-12-9-11-17(23-18)20(24)26-14-16

InchiKey: BNGFULGSXWTPID-UHFFFAOYSA-N

Formula: C22H35NO4

SMILES: CCCC(OC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1)C(C)C

Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.55		Crippen Method
logp	5.292		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpol	2396.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368792&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

https://www.chemeo.com/cid/17-301-8/2-6-Pyridinedicarboxylic-acid-2-methylhex-3-yl-2-4-4-trimethylpentyl-ester.pdf

Generated by Cheméo on 2024-10-12 05:22:00.244602198 +0000 UTC m=+3291382.881571448.

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