

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
rinsol	2396.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U368792&Units=SI

Legend

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

Latest version available from:

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

Generated by Cheméo on 2024-04-24 10:03:24.340534689 +0000 UTC m=+16242253.261112005.

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