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

Inchi: InChI=1S/C21H24ClNO4/c1-4-6-19(14(2)3)27-21(25)18-8-5-7-17(23-18)20(24)26-13-15-

InchiKey: RHLNEZMINYVKLL-UHFFFAOYSA-N

Formula: C21H24ClNO4

SMILES: CCCC(OC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1)C(C)C

Mol. weight [g/mol]: 389.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	5.073		Crippen Method
mcvol	296.330	ml/mol	McGowan Method
rinpol	2785.00		NIST Webbook
rinpol	2785.00		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=U369140&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

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