2,6-Pyridinedicarboxylic acid, di(4-chlorobenzyl) ester

Inchi: InChI=1S/C21H15Cl2NO4/c22-16-8-4-14(5-9-16)12-27-20(25)18-2-1-3-19(24-18)21(26)2

InchiKey: JTWHVQWGRBSVLL-UHFFFAOYSA-N

Formula: C21H15Cl2NO4

SMILES: O=C(OCc1ccc(Cl)cc1)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1

Mol. weight [g/mol]: 416.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	5.102		Crippen Method
mcvol	284.810	ml/mol	McGowan Method
rinpol	3300.00		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=U369146&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