2,6-Pyridinedicarboxylic acid, butyl 4-chlorobenzyl ester

Inchi: InChI=1S/C18H18ClNO4/c1-2-3-11-23-17(21)15-5-4-6-16(20-15)18(22)24-12-13-7-9-14(

InchiKey: OAHUOSQBJNRNGD-UHFFFAOYSA-N

Formula: C18H18ClNO4

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

Mol. weight [g/mol]: 347.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.049		Crippen Method
mcvol	254.060	ml/mol	McGowan Method
rinpol	2694.00		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=U369138&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