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

Inchi: InChI=1S/C18H18ClNO4/c1-12(2)10-23-17(21)15-4-3-5-16(20-15)18(22)24-11-13-6-8-14

InchiKey: QVYPDOGXWZDTLA-UHFFFAOYSA-N

Formula: C18H18ClNO4

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

Mol. weight [g/mol]: 347.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	3.905		Crippen Method
mcvol	254.060	ml/mol	McGowan Method
rinpol	2634.00		NIST Webbook

Sources

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=U369137&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices