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

Inchi: InChI=1S/C19H20ClNO4/c1-2-3-4-12-24-18(22)16-6-5-7-17(21-16)19(23)25-13-14-8-10-

InchiKey: XHGRRMRAPNPAPO-UHFFFAOYSA-N

Formula: C19H20ClNO4

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

Mol. weight [g/mol]: 361.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	4.439		Crippen Method
mcvol	268.150	ml/mol	McGowan Method
rinpol	2796.00		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=U369139&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