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

Inchi: InChI=1S/C21H24ClNO4/c1-2-3-4-5-6-14-26-20(24)18-8-7-9-19(23-18)21(25)27-15-16-1

InchiKey: ZQUKOGMMIFYMAO-UHFFFAOYSA-N

Formula: C21H24ClNO4

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

Mol. weight [g/mol]: 389.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.219		Crippen Method
mcvol	296.330	ml/mol	McGowan Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		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=U369142&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.