2,6-Pyridinedicarboxylic acid, 3,5-dichlorobenzyl heptyl ester

Inchi: InChI=1S/C21H23Cl2NO4/c1-2-3-4-5-6-10-27-20(25)18-8-7-9-19(24-18)21(26)28-14-15-

InchiKey: QOXSHOFQCIZJET-UHFFFAOYSA-N

Formula: C21H23Cl2NO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1

Mol. weight [g/mol]: 424.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.71		Crippen Method
logp	5.873		Crippen Method
mcvol	308.570	ml/mol	McGowan Method
rinpol	3074.00		NIST Webbook
rinpol	3074.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369106&Units=SI

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

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.