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

Inchi: InChI=1S/C22H25Cl2NO4/c1-2-3-4-5-6-7-11-28-21(26)19-9-8-10-20(25-19)22(27)29-15-

InchiKey: YEXSNDDYQQYEKS-UHFFFAOYSA-N

Formula: C22H25Cl2NO4

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

Mol. weight [g/mol]: 438.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.13		Crippen Method
logp	6.263		Crippen Method
mcvol	322.660	ml/mol	McGowan Method
rinpol	3137.00		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=U369107&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

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