2,6-Pyridinedicarboxylic acid, di(2-chlorophenyl) ester

Inchi: InChI=1S/C19H11Cl2NO4/c20-12-6-1-3-10-16(12)25-18(23)14-8-5-9-15(22-14)19(24)26-

InchiKey: FZHPIEDUWMUXPR-UHFFFAOYSA-N

Formula: C19H11Cl2NO4

SMILES: O=C(Oc1ccccc1Cl)c1cccc(C(=O)Oc2ccccc2Cl)n1

Mol. weight [g/mol]: 388.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	4.827		Crippen Method
mcvol	256.630	ml/mol	McGowan Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		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=U369133&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.