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

Inchi: InChI=1S/C16H13Cl2NO4/c1-2-22-15(20)13-4-3-5-14(19-13)16(21)23-9-10-6-11(17)8-12

InchiKey: AUBHKNTVZYWLJY-UHFFFAOYSA-N

Formula: C16H13Cl2NO4

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

Mol. weight [g/mol]: 354.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	3.922		Crippen Method
mcvol	238.120	ml/mol	McGowan Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369102&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.