

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

Inchi:	InChI=1S/C20H21Cl2NO4/c1-2-3-4-5-9-26-19(24)17-7-6-8-18(23-17)20(25)27-13-14-10-
InchiKey:	NZTGFIHPUCXMNU-UHFFFAOYSA-N
Formula:	C20H21Cl2NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1
Mol. weight [g/mol]:	410.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	5.482		Crippen Method
mcvol	294.480	ml/mol	McGowan Method
rinsol	2999.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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