

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

Inchi:	InChI=1S/C23H27Cl2NO4/c1-2-3-4-5-6-7-8-12-29-22(27)20-10-9-11-21(26-20)23(28)30-
InchiKey:	GWWGYKDCICSRRI-UHFFFAOYSA-N
Formula:	C23H27Cl2NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCc2cc(Cl)cc(Cl)c2)n1
Mol. weight [g/mol]:	452.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.55		Crippen Method
logp	6.653		Crippen Method
mcvol	336.750	ml/mol	McGowan Method
rinpola	3197.00		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=U369108&Units=SI

Legend

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

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