

2,6-Pyridinedicarboxylic acid, 4-chlorobenzyl nonyl ester

Inchi:	InChI=1S/C23H28ClNO4/c1-2-3-4-5-6-7-8-16-28-22(26)20-10-9-11-21(25-20)23(27)29-1
InchiKey:	FCJQLWGLHFJGDT-UHFFFAOYSA-N
Formula:	C23H28ClNO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]:	417.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	5.999		Crippen Method
mcvol	324.510	ml/mol	McGowan Method
rinpola	3119.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U369144&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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