

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

Inchi:	InChI=1S/C24H30ClNO4/c1-2-3-4-5-6-7-8-9-17-29-23(27)21-11-10-12-22(26-21)24(28)3
InchiKey:	GHXZRLCTCGUNLE-UHFFFAOYSA-N
Formula:	C24H30ClNO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]:	431.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	6.389		Crippen Method
mcvol	338.600	ml/mol	McGowan Method
rinpole	3180.00		NIST Webbook
rinpole	3180.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369145&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
rinpole:	Non-polar retention indices

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