

2,6-Pyridinedicarboxylic acid, 2-chlorophenyl hexyl ester

Inchi:	InChI=1S/C19H20ClNO4/c1-2-3-4-7-13-24-18(22)15-10-8-11-16(21-15)19(23)25-17-12-6
InchiKey:	COILYFCLRRXTDE-UHFFFAOYSA-N
Formula:	C19H20ClNO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2Cl)n1
Mol. weight [g/mol]:	361.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.34		Crippen Method
logp	4.691		Crippen Method
mcvol	268.150	ml/mol	McGowan Method
rinsol	2750.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369132&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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