

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

Inchi:	InChI=1S/C18H18ClNO4/c1-12(2)10-23-17(21)15-4-3-5-16(20-15)18(22)24-11-13-6-8-14
InchiKey:	QVYPDOGXWZDTLA-UHFFFAOYSA-N
Formula:	C18H18ClNO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]:	347.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	3.905		Crippen Method
mcvol	254.060	ml/mol	McGowan Method
rinsol	2634.00		NIST Webbook

Sources

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=U369137&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/68-901-6/2-6-Pyridinedicarboxylic-acid-4-chlorobenzyl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-18 21:41:45.679977112 +0000 UTC m=+15765754.600554437.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.