

2,6-Pyridinedicarboxylic acid, di(4-chlorobenzyl) ester

Inchi: InChI=1S/C21H15Cl2NO4/c22-16-8-4-14(5-9-16)12-27-20(25)18-2-1-3-19(24-18)21(26)2
InchiKey: JTWHVQWGRBSVLL-UHFFFAOYSA-N
Formula: C21H15Cl2NO4
SMILES: O=C(OCc1ccc(Cl)cc1)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]: 416.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	5.102		Crippen Method
mcvol	284.810	ml/mol	McGowan Method
rinpola	3300.00		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=U369146&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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