

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

Inchi: InChI=1S/C17H16ClNO4/c1-2-10-22-16(20)14-4-3-5-15(19-14)17(21)23-11-12-6-8-13(18)
InchiKey: OXYAIBJUIVZDGH-UHFFFAOYSA-N
Formula: C17H16ClNO4
SMILES: CCCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]: 333.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	3.659		Crippen Method
mcvol	239.970	ml/mol	McGowan Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369136&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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