

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

Inchi: InChI=1S/C19H20ClNO4/c1-2-3-4-12-24-18(22)16-6-5-7-17(21-16)19(23)25-13-14-8-10-
InchiKey: XHGRRMRAPNPAPO-UHFFFAOYSA-N
Formula: C19H20ClNO4
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Cl)cc2)n1
Mol. weight [g/mol]: 361.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	4.439		Crippen Method
mcvol	268.150	ml/mol	McGowan Method
rinpol	2796.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U369139&Units=SI>

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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