2,6-Pyridinedicarboxylic acid, 2-methylphenyl pentyl ester

Inchi: InChI=1S/C19H21NO4/c1-3-4-7-13-23-18(21)15-10-8-11-16(20-15)19(22)24-17-12-6-5-9

InchiKey: DWMHZIFIBOGFLW-UHFFFAOYSA-N

Formula: C19H21NO4

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)n1

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	3.956		Crippen Method
mcvol	255.910	ml/mol	McGowan Method
rinpol	2547.00		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=U369122&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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