2,6-Pyridinedicarboxylic acid, heptyl neopentyl ester

Inchi: InChI=1S/C19H29NO4/c1-5-6-7-8-9-13-23-17(21)15-11-10-12-16(20-15)18(22)24-14-19(

InchiKey: DQUBKWQWKZHKTH-UHFFFAOYSA-N

Formula: C19H29NO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	4.412		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2321.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369003&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices