2,6-Pyridinedicarboxylic acid, di(2-methylpentyl) ester

Inchi: InChI=1S/C19H29NO4/c1-5-8-14(3)12-23-18(21)16-10-7-11-17(20-16)19(22)24-13-15(4)

InchiKey: CSJACVWNPZUZQI-UHFFFAOYSA-N

Formula: C19H29NO4

SMILES: CCCC(C)COC(=O)c1cccc(C(=O)OCC(C)CCC)n1

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.268		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2336.00		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=U369099&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