2,6-Pyridinedicarboxylic acid, di(5-methoxy-3-methylpent-2-yl) ester

Inchi: InChI=1S/C21H33NO6/c1-14(10-12-25-5)16(3)27-20(23)18-8-7-9-19(22-18)21(24)28-17(

InchiKey: CBKOKKKTSKEAOK-UHFFFAOYSA-N

Formula: C21H33NO6

SMILES: COCCC(C)C(C)OC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1

Mol. weight [g/mol]: 395.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	3.517		Crippen Method
mcvol	319.590	ml/mol	McGowan Method
rinpol	2606.00		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=U369181&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