2,6-Pyridinedicarboxylic acid, ethyl 5-methoxy-3-methylpent-2-yl ester

Inchi: InChI=1S/C16H23NO5/c1-5-21-15(18)13-7-6-8-14(17-13)16(19)22-12(3)11(2)9-10-20-4/h

InchiKey: VUEDDNJBHAYZCU-UHFFFAOYSA-N

Formula: C16H23NO5

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

Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.476		Crippen Method
mcvol	243.270	ml/mol	McGowan Method
rinpol	2152.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369170&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices