2,6-Pyridinedicarboxylic acid, ethyl neopentyl ester

Inchi: InChI=1S/C14H19NO4/c1-5-18-12(16)10-7-6-8-11(15-10)13(17)19-9-14(2,3)4/h6-8H,5,9
InchiKey: BRYCICNMTNYUMV-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.461		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinpol	1834.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368997&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