2,6-Pyridinedicarboxylic acid, 2-ethylbutyl isobutyl ester

Inchi: InChI=1S/C17H25NO4/c1-5-13(6-2)11-22-17(20)15-9-7-8-14(18-15)16(19)21-10-12(3)4/l
InchiKey: YABHOZSPUHEOID-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCC(CC)COC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.487		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2157.00		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=U369038&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

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