2,6-Pyridinedicarboxylic acid, di(3-methylbutyl) ester

Inchi: InChI=1S/C17H25NO4/c1-12(2)8-10-21-16(19)14-6-5-7-15(18-14)17(20)22-11-9-13(3)4/h

InchiKey: LLTUXTPOCRCNJA-UHFFFAOYSA-N

Formula: C17H25NO4

SMILES: CC(C)CCOC(=O)c1cccc(C(=O)OCCC(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	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368331&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.