2,6-Pyridinedicarboxylic acid, ethyl 2-methylpentyl ester

Inchi: InChI=1S/C15H21NO4/c1-4-7-11(3)10-20-15(18)13-9-6-8-12(16-13)14(17)19-5-2/h6,8-9,

InchiKey: BIVCIXIIBULAPH-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: CCCC(C)COC(=O)c1cccc(C(=O)OCC)n1

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.851		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		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=U369080&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

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