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

Inchi: InChI=1S/C21H33NO4/c1-4-6-7-8-9-10-15-25-20(23)18-13-11-14-19(22-18)21(24)26-16-

InchiKey: NMKXLXFTKUDUGQ-UHFFFAOYSA-N

Formula: C21H33NO4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CCC)n1

Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	5.192		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinpol	2583.00		NIST Webbook
rinpol	2583.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369088&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.