2,6-Pyridinedicarboxylic acid, 4-octyl propyl ester

Inchi: InChI=1S/C18H27NO4/c1-4-7-10-14(9-5-2)23-18(21)16-12-8-11-15(19-16)17(20)22-13-6

InchiKey: XEKQAMDKWNJZRL-UHFFFAOYSA-N

Formula: C18H27NO4

SMILES: CCCCC(CCC)OC(=O)c1cccc(C(=O)OCCC)n1

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	4.164		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook

Sources

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=U368832&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.