2,6-Pyridinedicarboxylic acid, di(2-octyl) ester

Inchi: InChI=1S/C23H37NO4/c1-5-7-9-11-14-18(3)27-22(25)20-16-13-17-21(24-20)23(26)28-19

InchiKey: PCNJITYEUZXFRH-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCC(C)OC(=O)c1cccc(C(=O)OC(C)CCCCCC)n1

Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.81		Crippen Method
logp	6.113		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368313&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.