2,6-Pyridinedicarboxylic acid, hexadecyl 2-pentyl ester

Inchi: InChI=1S/C28H47NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-23-32-27(30)25-21-19-

InchiKey: KXCKYFCDHIAVPP-UHFFFAOYSA-N

Formula: C28H47NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCC)n1

Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.79		Crippen Method
logp	8.065		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		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=U368346&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.