2,6-Pyridinedicarboxylic acid, dodecyl nonyl ester

Inchi: InChI=1S/C28H47NO4/c1-3-5-7-9-11-12-13-15-17-19-24-33-28(31)26-22-20-21-25(29-26

InchiKey: KQAAUMGNQILLTL-UHFFFAOYSA-N

Formula: C28H47NO4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCC)n1

Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.68		Crippen Method
logp	8.067		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinpol	3207.00		NIST Webbook
rinpol	3207.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368826&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.