2,6-Pyridinedicarboxylic acid, hexadecyl octyl ester

Inchi: InChI=1S/C31H53NO4/c1-3-5-7-9-11-12-13-14-15-16-17-18-20-22-27-36-31(34)29-25-23

InchiKey: IHQAXQUOSULHQV-UHFFFAOYSA-N

Formula: C31H53NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCC)n1

Mol. weight [g/mol]: 503.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.93		Crippen Method
logp	9.237		Crippen Method
mcvol	448.750	ml/mol	McGowan Method
rinpol	3439.00		NIST Webbook
rinpol	3439.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369035&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

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