2,6-Pyridinedicarboxylic acid, octadecyl pentyl ester

Inchi: InChI=1S/C30H51NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-26-35-30(33)28-

InchiKey: XYJYOWDONQIJFZ-UHFFFAOYSA-N

Formula: C30H51NO4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1

Mol. weight [g/mol]: 489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.51		Crippen Method
logp	8.847		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpol	3371.00		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=U368296&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

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