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

Inchi: InChI=1S/C30H51NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-34-29(32)27-
InchiKey: ZSBKZXBCRUOJCT-UHFFFAOYSA-N
Formula: C30H51NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCC)n1
Mol. weight [g/mol]: 489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	8.845		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook

Sources

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=U368348&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.