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

Inchi: InChI=1S/C25H41NO4/c1-4-6-7-8-9-10-11-12-13-14-15-20-29-24(27)22-18-16-19-23(26-

InchiKey: FTYNEPDEDSAZQX-UHFFFAOYSA-N

Formula: C25H41NO4

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

Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.53		Crippen Method
logp	6.895		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368343&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.