2,6-Pyridinedicarboxylic acid, decyl heptyl ester

Inchi: InChI=1S/C24H39NO4/c1-3-5-7-9-10-11-13-15-20-29-24(27)22-18-16-17-21(25-22)23(26

InchiKey: DEHPLIBOHLQEIR-UHFFFAOYSA-N

Formula: C24H39NO4

SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCC)n1

Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	6.506		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
rinpol	2929.00		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=U368810&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