2,6-Pyridinedicarboxylic acid, decyl 4-octyl ester

Inchi: InChI=1S/C25H41NO4/c1-4-7-9-10-11-12-13-14-20-29-24(27)22-18-15-19-23(26-22)25(2

InchiKey: OEXMSFCWIMYIRK-UHFFFAOYSA-N

Formula: C25H41NO4

SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)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	2862.00		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=U368839&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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