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

Inchi: InChI=1S/C23H37NO4/c1-4-7-9-10-11-12-18-27-22(25)20-16-13-17-21(24-20)23(26)28-1
InchiKey: JYKAXUOXFBWKGL-UHFFFAOYSA-N
Formula: C23H37NO4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)n1
Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69		Crippen Method
logp	6.115		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368837&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.