2,6-Pyridinedicarboxylic acid, decyl 2-methylbutyl ester

Inchi: InChI=1S/C22H35NO4/c1-4-6-7-8-9-10-11-12-16-26-21(24)19-14-13-15-20(23-19)22(25)
InchiKey: LIUXRBRHGCSNQW-UHFFFAOYSA-N
Formula: C22H35NO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)n1
Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.92		Crippen Method
logp	5.582		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpol	2700.00		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=U369066&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