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

Inchi: InChI=1S/C19H29NO4/c1-4-6-8-9-11-15(3)24-19(22)17-13-10-12-16(20-17)18(21)23-14-
InchiKey: DAEUGOWUFJXIDI-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCC(C)OC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.02		Crippen Method
logp	4.554		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2339.00		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=U368300&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

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