2,6-Pyridinedicarboxylic acid, hexyl 3-methylbutyl ester

Inchi: InChI=1S/C18H27NO4/c1-4-5-6-7-12-22-17(20)15-9-8-10-16(19-15)18(21)23-13-11-14(2
InchiKey: UVPTVSLEIRHJBN-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.022		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2321.00		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=U368318&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