2,6-Pyridinedicarboxylic acid, hexyl isopropyl ester

Inchi: InChI=1S/C16H23NO4/c1-4-5-6-7-11-20-15(18)13-9-8-10-14(17-13)16(19)21-12(2)3/h8-1

InchiKey: MNUAWWNWLRWPAZ-UHFFFAOYSA-N

Formula: C16H23NO4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(C)C)n1

Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.384		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpol	2096.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369151&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