2,6-Pyridinedicarboxylic acid, ethyl hexyl ester

Inchi: InChI=1S/C15H21NO4/c1-3-5-6-7-11-20-15(18)13-10-8-9-12(16-13)14(17)19-4-2/h8-10H
InchiKey: FQWTXMYTQXQJKK-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC)n1
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	2.995		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpol	2201.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368772&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices