2,6-Pyridinedicarboxylic acid, ethyl heptyl ester

Inchi: InChI=1S/C16H23NO4/c1-3-5-6-7-8-12-21-16(19)14-11-9-10-13(17-14)15(18)20-4-2/h9-1
InchiKey: LQYSCKJNVBZFOU-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCC)n1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.385		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369022&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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