2,6-Pyridinedicarboxylic acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C16H12N2O4/c1-2-21-15(19)13-4-3-5-14(18-13)16(20)22-12-8-6-11(10-17)7-9

InchiKey: HQQSXOVICWRKOL-UHFFFAOYSA-N

Formula: C16H12N2O4

SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)n1

Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	2.349		Crippen Method
mcvol	215.020	ml/mol	McGowan Method
rinpol	2555.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369134&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