

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
rinpola	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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/43-166-0/2-6-Pyridinedicarboxylic-acid-4-cyanophenyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-26 09:23:56.440185219 +0000 UTC m=+16412685.360762534.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.