2,3-Pyridinedicarboxylic anhydride

Other names:	Pyridine-2,3-dicarboxylic anhydride
	Furo[3,4-b]pyridine-5,7-dione
Inchi:	InChI=1S/C7H3NO3/c9-6-4-2-1-3-8-5(4)7(10)11-6/h1-3H
InchiKey:	MCQOWYALZVKMAR-UHFFFAOYSA-N
Formula:	C7H3NO3
SMILES:	O=C1OC(=O)c2ncccc21
Mol. weight [g/mol]:	149.10
CAS:	699-98-9

Physical Properties

Property code	Value	Unit	Source
ea	1.39 ± 0.09	eV	NIST Webbook
ie	10.50 ± 0.10	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	0.392		Crippen Method
mcvol	93.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C699989&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

ea:	Electron affinity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume