3,4-Pyridinedicarboxylic acid, dimethyl ester

Other names:	Cinchomeronic acid, dimethyl ester
	Dimethyl 3,4-pyridinedicarboxylate
	Dimethyl pyridine-3,4-dicarboxylate
Inchi:	InChI=1S/C9H9NO4/c1-13-8(11)6-3-4-10-5-7(6)9(12)14-2/h3-5H,1-2H3
InchiKey:	AUQUSBAFIHOGHK-UHFFFAOYSA-N
Formula:	C9H9NO4
SMILES:	COC(=O)c1ccncc1C(=O)OC
Mol. weight [g/mol]:	195.17
CAS:	1796-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	0.655		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
rinpol	1502.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1796834&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

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