

3,4-Pyridinedicarboxylic acid

Other names:	Pyridine-3,4-dicarboxylic acid Chinchomeric acid Cinchomeric acid
Inchi:	InChI=1S/C7H5NO4/c9-6(10)4-1-2-8-3-5(4)7(11)12/h1-3H,(H,9,10)(H,11,12)
InchiKey:	MUYSADWCWFFZKR-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1ccncc1C(=O)O
Mol. weight [g/mol]:	167.12
CAS:	490-11-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.36		Crippen Method
logp	0.478		Crippen Method
mcvol	110.590	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C490119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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