

2,6-Dihydroxyisonicotinic acid

Other names:	Citrazinic acid 4-Pyridinecarboxylic acid, 1,2-dihydro-6-hydroxy-2-oxo- Isonicotinic acid, 2,6-dihydroxy- 2,6-Dihydroxy-4-carboxypyridine 2,6-Dihydroxy-4-pyridinecarboxylic acid 4-Pyridinecarboxylic acid, 2,6-dihydroxy- Kyselina citrazinova
Inchi:	InChI=1S/C6H5NO4/c8-4-1-3(6(10)11)2-5(9)7-4/h1-2H,(H,10,11)(H2,7,8,9)
InchiKey:	CSGQJHQYWJLPKY-UHFFFAOYSA-N
Formula:	C6H5NO4
SMILES:	O=C(O)c1cc(O)nc(O)c1
Mol. weight [g/mol]:	155.11
CAS:	99-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.39		Crippen Method
logp	0.191		Crippen Method
mcvol	100.800	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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