

# 4-oxopyran-2,6-dicarboxylic acid

<b>Inchi:</b>	InChI=1S/C7H4O6/c8-3-1-4(6(9)10)13-5(2-3)7(11)12/h1-2H,(H,9,10)(H,11,12)
<b>InchiKey:</b>	PBAYDYUZOSNJGU-UHFFFAOYSA-N
<b>Formula:</b>	C7H4O6
<b>SMILES:</b>	O=C(O)c1cc(=O)cc(C(=O)O)o1
<b>Mol. weight [g/mol]:</b>	184.10

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Aqueous Solubility Prediction Method
logp	0.036		Crippen Method
mcvol	112.350	ml/mol	McGowan Method

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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