4-oxopyran-2,6-dicarboxylic acid

Inchi: 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)
InchiKey: PBAYDYUZOSNJGU-UHFFFAOYSA-N
Formula: C7H4O6
SMILES: O=C(O)c1cc(=O)cc(C(=O)O)o1
Mol. weight [g/mol]: 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/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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