Acetophenone, 2,3,4-trihydroxy-

Inchi: InChI=1S/C8H8O4/c1-4(9)5-2-3-6(10)8(12)7(5)11/h2-3,10-12H,1H3
InchiKey: XIROXSOOOAZHLL-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: CC(=O)c1ccc([O])c([O])c1[O]
Mol. weight [g/mol]: 168.15
CAS: 29477-54-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.66		Crippen Method
logp	2.321		Crippen Method
mcvol	112.550	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29477541&Units=SI

Legend

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