

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:	XIROXS000AZHLL-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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/88-240-8/Acetophenone-2-3-4-trihydroxy.pdf>

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