# 3-hydroxy-6-methyl-2(2H)-pyranone

**Inchi:** InChI=1S/C6H6O3/c1-4-2-3-5(7)6(8)9-4/h2-3,7H,1H3
**InchiKey:** MJIACMMODTYUHG-UHFFFAOYSA-N
**Formula:** C6H6O3
**SMILES:** Cc1ccc(O)c(=O)o1
**Mol. weight [g/mol]:** 126.11

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.65 | | Crippen Method |
| logp | 0.654 | | Crippen Method |
| mcvol | 89.250 | ml/mol | McGowan Method |
| rinpol | 1047.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| ripol | 2035.00 | | NIST Webbook |
| ripol | 2035.00 | | NIST Webbook |
| ripol | 2035.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R225611&Units=SI
**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

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices