

# Coumarin, 5-hydroxy-

**Inchi:** InChI=1S/C9H6O3/c10-7-2-1-3-8-6(7)4-5-9(11)12-8/h1-5,10H  
**InchiKey:** CDHSCTCRBLLCBBJ-UHFFFAOYSA-N  
**Formula:** C9H6O3  
**SMILES:** O=c1ccc2c(O)cccc2o1  
**Mol. weight [g/mol]:** 162.14  
**CAS:** 6093-67-0

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.98   |        | Crippen Method |
| logp          | 1.499   |        | Crippen Method |
| mcvol         | 112.060 | ml/mol | McGowan Method |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6093670&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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