

# 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl)-

**Other names:** 5-Hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one

Salvigenin

**Inchi:** InChI=1S/C18H16O6/c1-21-11-6-4-10(5-7-11)13-8-12(19)16-14(24-13)9-15(22-2)18(23-3)

**InchiKey:** QCDYOIZVELGOLZ-UHFFFAOYSA-N

**Formula:** C18H16O6

**SMILES:** COc1ccc(-c2cc(=O)c3c(O)c(OC)c(OC)cc3o2)cc1

**Mol. weight [g/mol]:** 328.32

**CAS:** 19103-54-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	3.191		Crippen Method
mcvol	232.720	ml/mol	McGowan Method
rinpol	3232.60		NIST Webbook

## Sources

**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>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19103549&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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