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

**Other names:** Flavone, 4',5,6,7-tetramethoxy-
Scutellarein tetramethyl ether
Tetra-O-methylscutellarein
Tetramethyl-O-scutellarin
4',5,6,7-Tetramethoxyflavone
Flavone, 5,6,7,4'-tetramethoxy

**Inchi:** InChI=1S/C19H18O6/c1-21-12-7-5-11(6-8-12)14-9-13(20)17-15(25-14)10-16(22-2)18(23

**InchiKey:** URSUMOWUGDXZHU-UHFFFAOYSA-N

**Formula:** C19H18O6

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

**Mol. weight [g/mol]:** 342.34

**CAS:** 1168-42-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -9.51 | | Crippen Method |
| logp | 3.494 | | Crippen Method |
| mcvol | 246.810 | ml/mol | McGowan Method |
| rinpol | 3249.00 | | NIST Webbook |
| rinpol | 3250.30 | | NIST Webbook |
| rinpol | 3186.00 | | NIST Webbook |
| rinpol | 3186.00 | | NIST Webbook |
| rinpol | 3249.00 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1168429&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

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