

# 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
mcpvol	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](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

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

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