

# 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-

Other names:

Biochanin B  
Formononetin  
Formononetol  
Isoflavone, 7-hydroxy-4'-methoxy-  
7-Hydroxy-4'-methoxyisoflavone  
7-hydroxy-3-(4-methoxyphenyl)-4-benzopyrone  
7-Hydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one

Inchi:

InChI=1S/C16H12O4/c1-19-12-5-2-10(3-6-12)14-9-20-15-8-11(17)4-7-13(15)16(14)18/h2

InchiKey:

HKQYGTCOTHHOMP-UHFFFAOYSA-N

Formula:

C16H12O4

SMILES:

COc1ccc(-c2coc3cc(O)ccc3c2=O)cc1

Mol. weight [g/mol]:

268.26

CAS:

485-72-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.70		Crippen Method
logp	3.174		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
rinpol	2869.40		NIST Webbook
rinpol	2869.40		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=C485723&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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