

# 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)-6-methoxy-

Other names:

Flavone, 4',5,7-trihydroxy-6-methoxy-

Dinatin

Hispidulin

4',5,7-Trihydroxy-6-methoxyflavone

6-O-Methylapigenin

Hispedulin

Inchi:

InChI=1S/C16H12O6/c1-21-16-11(19)7-13-14(15(16)20)10(18)6-12(22-13)8-2-4-9(17)5-3

InchiKey:

IHFBPDAQLQOCBX-UHFFFAOYSA-N

Formula:

C16H12O6

SMILES:

COc1c(O)cc2oc(-c3ccc(O)cc3)cc(=O)c2c1O

Mol. weight [g/mol]:

300.26

CAS:

1447-88-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	2.585		Crippen Method
mcvol	204.540	ml/mol	McGowan Method
rmpol	3150.60		NIST Webbook
rmpol	3150.60		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=C1447887&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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