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
rinpol	3150.60		NIST Webbook
rinpol	3150.60		NIST Webbook

Sources

Crippen Method: 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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices