4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-phenyl-

Other names: Flavone, 5-hydroxy-7-methoxy-
Tectochrysin
5-Hydroxy-7-methoxyflavone
7-Methoxy-5-hydroxyflavone

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

InchiKey: IRZVHDLBAYNPCT-UHFFFAOYSA-N

Formula: C16H12O4

SMILES: COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1

Mol. weight [g/mol]: 268.26

CAS: 520-28-5

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	2543.00		NIST Webbook
rinpol	2628.20		NIST Webbook
rinpol	2543.00		NIST Webbook
rinpol	2628.20		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C520285&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