

# Osthole

**Other names:**

2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methyl-2-buten-1-yl)-  
2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methyl-2-butenyl)-  
7-Methoxy-8-(3-methyl-2-butenyl)-coumarin  
7-Methoxy-8-isopentenylcoumarin  
7-methoxy-8-(3-methylbut-2-en-1-yl)-2H-chromen-2-one  
8-(3-Methyl-2-butenyl)herniarin  
Coumarin, 7-methoxy-8-(3-methyl-2-butenyl)-  
NSC 31868  
Osthol  
Ostol  
Ostole

**Inchi:**

InChI=1S/C15H16O3/c1-10(2)4-7-12-13(17-3)8-5-11-6-9-14(16)18-15(11)12/h4-6,8-9H,7

**InchiKey:**

MBRLOUHOWLUMFF-UHFFFAOYSA-N

**Formula:**

C15H16O3

**SMILES:**

COc1ccc2ccc(=O)oc2c1CC=C(C)C

**Mol. weight [g/mol]:**

244.29

**CAS:**

484-12-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Estimated Solubility Method
log10ws	-4.31		Aqueous Solubility Prediction Method
logp	3.310		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
rinpol	2174.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2157.00		NIST Webbook
ripol	2942.00		NIST Webbook

ripol	2942.00		NIST Webbook
tf	356.65	K	Aqueous Solubility Prediction Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Solubility of osthole in a binary system of ethanol and water:** <https://www.doi.org/10.1016/j.fluid.2012.04.005>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

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

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C484128&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**ripol:** Non-polar retention indices

**ripol:** Polar retention indices

**tf:** Normal melting (fusion) point

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