# 2H-1-Benzopyran-2-one, 7-[(3,7-dimethyl-2,6-octadienyl)oxy]-, (E)-

**Other names:** Coumarin, 7-[(3,7-dimethyl-2,6-octadienyl)oxy]-, (E)-
(E)-7-((3,7-Dimethylocta-2,6-dien-1-yl)oxy)-2H-chromen-2-one
2H-1-Benzopyran-2-one, 7-[[(2E)-3,7-dimethyl-2,6-octadien-1-yl]oxy]-
Aurapten
7-Geranyloxycoumarin
Auraptene
Coumarin, 7-(geranyloxy)-

**Inchi:** InChI=1S/C19H22O3/c1-14(2)5-4-6-15(3)11-12-21-17-9-7-16-8-10-19(20)22-18(16)13-17

**InchiKey:** RSDDHGSKLOSQFK-RVDMUPIBSA-N

**Formula:** C19H22O3

**SMILES:** CC(C)=CCCC(C)=CCOc1ccc2ccc(=O)oc2c1

**Mol. weight [g/mol]:** 298.38

**CAS:** 495-02-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -10.03 | | Crippen Method |
| logp | 4.865 | | Crippen Method |
| mcvol | 244.360 | ml/mol | McGowan Method |
| rinpol | 2634.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C495023&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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

## Legend

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

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices