

# 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]-  
Auraptin  
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/ci9903071>

**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>

## 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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