

# Eupatorin

**Inchi:** InChI=1S/C18H16O7/c1-22-12-5-4-9(6-10(12)19)13-7-11(20)16-14(25-13)8-15(23-2)18(21)2  
**InchiKey:** KLAOKWJLUQKWIF-UHFFFAOYSA-N  
**Formula:** C18H16O7  
**SMILES:** COc1ccc(-c2cc(=O)c3c(O)c(OC)c(OC)cc3o2)cc1O  
**Mol. weight [g/mol]:** 344.32  
**CAS:** 855-96-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	2.897		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
rinpola	3422.30		NIST Webbook
rinpola	3422.30		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C855969&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/81-785-1/Eupatorin.pdf>

Generated by Cheméo on 2024-04-19 21:36:08.14953768 +0000 UTC m=+15851817.070115002.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.