

# Jaceosidin

**Inchi:** InChI=1S/C17H14O7/c1-22-13-5-8(3-4-9(13)18)12-6-10(19)15-14(24-12)7-11(20)17(23-21)16  
**InchiKey:** GLAAQZFBFGEBPS-UHFFFAOYSA-N  
**Formula:** C17H14O7  
**SMILES:** COc1cc(-c2cc(=O)c3c(O)c(OC)c(O)cc3o2)ccc1O  
**Mol. weight [g/mol]:** 330.29  
**CAS:** 18085-97-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.92		Crippen Method
logp	2.594		Crippen Method
mcvol	224.500	ml/mol	McGowan Method
rinpol	3202.30		NIST Webbook
rinpol	3202.30		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=C18085977&Units=SI>

## 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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