

# (Z)-Cnidimine

**Inchi:** InChI=1S/C21H22O7/c1-6-11(2)20(24)27-18-16-14(25-19(18)21(4,5)28-12(3)22)9-7-13-8  
**InchiKey:** FFCDTHIJWHJUQJ-WDZFZDKYSA-N  
**Formula:** C21H22O7  
**SMILES:** CC=C(C)C(=O)OC1c2c(ccc3ccc(=O)oc23)OC1C(C)(C)OC(C)=O  
**Mol. weight [g/mol]:** 386.40  
**CAS:** 15591-75-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.28		Crippen Method
logp	3.446		Crippen Method
mcvol	280.860	ml/mol	McGowan Method
rinpol	2822.40		NIST Webbook
rinpol	2822.40		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=C15591750&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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