

# (1R,9S)-1-Acetoxy-N-acetyl-1,9-dihydro-anhydron

**Inchi:** InChI=1S/C25H27NO10/c1-13(27)26-9-8-15-10-18-22(35-12-34-18)23(33-5)20(15)25(26)  
**InchiKey:** JYLSYDBZXRABOF-RUZDIDTESA-N  
**Formula:** C25H27NO10  
**SMILES:** COc1ccc(CC2(OC(C)=O)c3c(cc4c(c3OC)OCO4)CCN2C(C)=O)c(C(=O)O)c1OC  
**Mol. weight [g/mol]:** 501.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	2.502		Crippen Method
mcvol	349.650	ml/mol	McGowan Method
rinpola	3848.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R330733&Units=SI>  
**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>

## Legend

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

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