

# Acetylerucifoline

**Inchi:** InChI=1S/C20H25NO7/c1-4-13-9-20(11-26-12(2)22)19(3,28-20)18(24)25-10-14-5-7-21-8  
**InchiKey:** PSLAXCVGXXVNFJ-VFCKIOPBSA-N  
**Formula:** C20H25NO7  
**SMILES:** CC=C1CC2(COC(C)=O)OC2(C)C(=O)OCC2=CCN3CCC(OC1=O)C23  
**Mol. weight [g/mol]:** 391.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	0.897		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
rinpol	2610.00		NIST Webbook
rinpol	2680.00		NIST Webbook
rinpol	2610.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178080&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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