

# Dicumarol Me

**Inchi:** InChI=1S/C21H16O6/c1-24-18-12-7-3-5-9-16(12)26-20(22)14(18)11-15-19(25-2)13-8-4-6  
**InchiKey:** RXKXACHXILQLBF-UHFFFAOYSA-N  
**Formula:** C21H16O6  
**SMILES:** COc1c(Cc2c(OC)c3ccccc3oc2=O)c(=O)oc2ccccc12  
**Mol. weight [g/mol]:** 364.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-13.73		Crippen Method
logp	3.507		Crippen Method
mcvol	255.530	ml/mol	McGowan Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook

## Sources

**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=R40023&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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