

# Coronarin E

**Inchi:** InChI=1S/C20H28O/c1-15-6-9-18-19(2,3)11-5-12-20(18,4)17(15)8-7-16-10-13-21-14-16/  
**InchiKey:** QXVXYNOIXUIXBI-BQYQJAHWSA-N  
**Formula:** C20H28O  
**SMILES:** C=C1CCC2C(C)(C)CCCC2(C)C1C=Cc1ccoc1  
**Mol. weight [g/mol]:** 284.44  
**CAS:** 117591-81-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.57		Crippen Method
logp	6.092		Crippen Method
mcvol	248.750	ml/mol	McGowan Method
rinpol	2135.60		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=C117591818&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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