

# Cinnamoylcocaine

**Inchi:** InChI=1S/C19H23NO4/c1-20-14-9-10-15(20)18(19(22)23-2)16(12-14)24-17(21)11-8-13-6  
**InchiKey:** MQIXMJWNEKUAOZ-DHZHZOJOSA-N  
**Formula:** C19H23NO4  
**SMILES:** COC(=O)C1C(OC(=O)C=Cc2ccccc2)CC2CCC1N2C  
**Mol. weight [g/mol]:** 329.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.267		Crippen Method
mcvol	253.650	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2480.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U247787&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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