

# m-Hydroxycocaine

**Inchi:** InChI=1S/C17H21NO5/c1-18-11-6-7-13(18)15(17(21)22-2)14(9-11)23-16(20)10-4-3-5-12  
**InchiKey:** IQXBUEUAOWARGT-UHFFFAOYSA-N  
**Formula:** C17H21NO5  
**SMILES:** COC(=O)C1C(OC(=O)c2cccc(O)c2)CC2CCC1N2C  
**Mol. weight [g/mol]:** 319.35  
**CAS:** 71387-58-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	1.573		Crippen Method
mcvol	235.640	ml/mol	McGowan Method
rinpola	2586.70		NIST Webbook
rinpola	2586.70		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C71387581&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)

## 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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