

# O-(4-Hydroxybenzoyl)tropine, O-methyl-

**Inchi:** InChI=1S/C16H21NO3/c1-17-12-5-6-13(17)10-15(9-12)20-16(18)11-3-7-14(19-2)8-4-11/  
**InchiKey:** JOROTINCCHPFDK-UHFFFAOYSA-N  
**Formula:** C16H21NO3  
**SMILES:** COc1ccc(C(=O)OC2CC3CCC(C2)N3C)cc1  
**Mol. weight [g/mol]:** 275.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.477		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2323.00		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=U374670&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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