

# 3«alpha»-Phenylacetoxytropane

**Inchi:** InChI=1S/C16H21NO2/c1-17-13-7-8-14(17)11-15(10-13)19-16(18)9-12-5-3-2-4-6-12/h2-  
**InchiKey:** DCINQANYMBYYCH-UHFFFAOYSA-N  
**Formula:** C16H21NO2  
**SMILES:** CN1C2CCC1CC(OC(=O)Cc1ccccc1)C2  
**Mol. weight [g/mol]:** 259.34  
**CAS:** 1690-22-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.398		Crippen Method
mcvol	208.240	ml/mol	McGowan Method
rinpol	2014.40		NIST Webbook
rinpol	2014.40		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1690228&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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