

# Carr's ketol, TMS

**Inchi:** InChI=1S/C15H22O3/c1-10(2)8-13(16)14-11(3)4-6-15(14,17)12-5-7-18-9-12/h5,7,9-11,14-15  
**InchiKey:** PLJLLELLRWAYEB-NILFDRSVSA-N  
**Formula:** C15H22O3  
**SMILES:** CC(C)CC(=O)C1C(C)CCC1(O)c1ccoc1  
**Mol. weight [g/mol]:** 250.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	3.129		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
rinpola	1764.00		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=R584806&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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