

# R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone (desmethylene-3-methyl-oxo-), ethylated

**InChI:** InChI=1S/C16H21NO4/c1-4-21-13-8-7-12/10-14(11-20-3)16(19)11(2)17-9-5-6-15(17)18/1  
**InChIKey:** MRQHCTHUENHKBV-UHFFFAOYSA-N

**Formula:** C<sub>16</sub>H<sub>21</sub>NO<sub>4</sub>

**SMILES:** CCOc1ccc(C(=O)C(C)N2CCCC2=O)cc1OC

**Mol. weight [g/mol]:** 291.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.288		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R290709&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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