

# 5-(Methylenedioxyphenyl)-2-pentenoyl pyrrolidide

**Inchi:** InChI=1S/C16H19NO3/c18-16(17-9-3-4-10-17)6-2-1-5-13-7-8-14-15(11-13)20-12-19-14/  
**InchiKey:** XZTCTKKANUDQCW-QHHAFSJGSA-N  
**Formula:** C16H19NO3  
**SMILES:** O=C(C=CCCc1ccc2c(c1)OCO2)N1CCCC1  
**Mol. weight [g/mol]:** 273.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.526		Crippen Method
mcvol	209.810	ml/mol	McGowan Method
rinsol	2572.00		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=R546042&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  
**rinsol:** Non-polar retention indices

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