

# (E)-5-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)pent-3-en-1-one

**Inchi:** InChI=1S/C17H21NO3/c19-17(18-10-4-1-5-11-18)7-3-2-6-14-8-9-15-16(12-14)21-13-20-19  
**InchiKey:** MJBOPSKIWRUIBB-NSCUHMNNSA-N  
**Formula:** C17H21NO3  
**SMILES:** O=C(CC=CCc1ccc2c(c1)OCO2)N1CCCCC1  
**Mol. weight [g/mol]:** 287.35  
**CAS:** 23512-55-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.917		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
rinpol	2601.80		NIST Webbook
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## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=C23512552&Units=SI>

## 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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