

# (E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)non-8-en-1-one

**Inchi:** InChI=1S/C21H29NO3/c23-21(22-14-8-5-9-15-22)11-7-4-2-1-3-6-10-18-12-13-19-20(16-20)  
**InchiKey:** FAXXHNWVMKTOFF-UXBLZVDNSA-N  
**Formula:** C21H29NO3  
**SMILES:** O=C(CCCCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1  
**Mol. weight [g/mol]:** 343.46  
**CAS:** 30505-89-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.782		Crippen Method
mcvol	280.260	ml/mol	McGowan Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=C30505896&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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