

# (2E,6E)-7-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-

**Inchi:** InChI=1S/C19H23NO3/c21-19(20-12-6-3-7-13-20)9-5-2-1-4-8-16-10-11-17-18(14-16)23-  
**InchiKey:** HFKLKVAMFMBFCX-KBXRYBNXSA-N  
**Formula:** C19H23NO3  
**SMILES:** O=C(C=CCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1  
**Mol. weight [g/mol]:** 313.39  
**CAS:** 147030-09-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.777		Crippen Method
mcvol	247.780	ml/mol	McGowan Method
rinpol	2999.30		NIST Webbook
rinpol	2999.30		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030099&Units=SI>  
**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)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/99-734-8/2E-6E-7-Benzo-d-1-3-dioxol-5-yl-1-piperidin-1-yl-hepta-2-6-dien-1-one.pdf>

Generated by Cheméo on 2024-04-19 19:02:27.732784354 +0000 UTC m=+15842596.653361685.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.