

# Benzylpiperazine-M (OH-) isomer-2, 2AC

**Inchi:** InChI=1S/C15H20N2O3/c1-12(18)17-9-7-16(8-10-17)11-14-5-3-4-6-15(14)20-13(2)19/h3  
**InchiKey:** JDIBNHDMHADMF-C-UHFFFAOYSA-N  
**Formula:** C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>  
**SMILES:** CC(=O)Oc1ccccc1CN1CCN(C(C)=O)CC1  
**Mol. weight [g/mol]:** 276.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.276		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2275.00		NIST Webbook
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## 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=R284318&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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