

# Butallylonal permethylated

**Inchi:** InChI=1S/C13H19BrN2O3/c1-6-8(2)13(7-9(3)14)10(17)15(4)12(19)16(5)11(13)18/h8H,3,  
**InchiKey:** GOCNAOAYIZROIY-UHFFFAOYSA-N  
**Formula:** C13H19BrN2O3  
**SMILES:** C=C(Br)CC1(C(C)CC)C(=O)N(C)C(=O)N(C)C1=O  
**Mol. weight [g/mol]:** 331.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.368		Crippen Method
mcvol	221.040	ml/mol	McGowan Method
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R387803&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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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