

# Butallylonal perethylated

**Inchi:** InChI=1S/C15H23BrN2O3/c1-6-10(4)15(9-11(5)16)12(19)17(7-2)14(21)18(8-3)13(15)20/  
**InchiKey:** BEUBFTHEVHCONL-UHFFFAOYSA-N  
**Formula:** C15H23BrN2O3  
**SMILES:** C=C(Br)CC1(C(C)CC)C(=O)N(CC)C(=O)N(CC)C1=O  
**Mol. weight [g/mol]:** 359.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	3.148		Crippen Method
mcvol	249.220	ml/mol	McGowan Method
rinpol	1739.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R387794&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**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

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