

# Gamabufotalin

**Other names:**

Bufa-20,22-dienolide, 3,11,14-trihydroxy-, (3«beta»,5«beta»,11«alpha»)-  
5«beta»-Bufa-20,22-dienolide, 3«beta»,11«alpha»,14-trihydroxy-  
Gamabufagin  
Gamabufogenin  
Gammabufotalin

**Inchi:**

3-«beta»,11-«alpha»,14-Trihydroxy-5-«beta»-bufa-20,22-dienolide

**InchiKey:**

FMTLOAVOGWSPEF-UHFFFAOYSA-N

**Formula:**

C<sub>24</sub>H<sub>34</sub>O<sub>5</sub>

**SMILES:**

CC12CCC(O)CC1CCC1C2C(O)CC2(C)C(c3ccc(=O)oc3)CCC12O

**Mol. weight [g/mol]:**

402.52

**CAS:**

465-11-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.01		Crippen Method
logp	3.213		Crippen Method
mcvol	311.170	ml/mol	McGowan Method

## Sources

**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>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C465112&Units=SI>

## Legend

**log10ws:**

Log10 of Water solubility in mol/l

**logp:**

Octanol/Water partition coefficient

**mcvol:**

McGowan's characteristic volume

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