

Bufotalin

Other names:	Bufa-20,22-dienolide, 16-(acetyloxy)-3,14-dihydroxy-, (3«beta»,5«beta»,16«beta»)-5«beta»-Bufa-20,22-dienolide, 3«beta»,14,16«beta»-trihydroxy-, 16-acetate Bufotaline
Inchi:	InChI=1S/C26H36O6/c1-15(27)32-21-13-26(30)20-6-5-17-12-18(28)8-10-24(17,2)19(20)
InchiKey:	VOZHMAYHYHEWBW-UHFFFAOYSA-N
Formula:	C26H36O6
SMILES:	CC(=O)OC1CC2(O)C3CCC4CC(O)CCC4(C)C3CCC2(C)C1c1ccc(=O)oc1
Mol. weight [g/mol]:	444.56
CAS:	471-95-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.44		Crippen Method
logp	3.784		Crippen Method
mcvol	340.920	ml/mol	McGowan Method

Sources

Crippen Method:	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=C471954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/86-643-3/Bufotalin.pdf>

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