

# 21-Hydroxypregn-4-en-3,20-dione, 20,21-methylboronate

**Inchi:** InChI=1S/C22H31BO3/c1-21-10-8-15(24)12-14(21)4-5-16-17-6-7-19(20-13-25-23(3)26-2  
**InchiKey:** BAJZWLGBRKRURW-BMVMDBOLSA-N  
**Formula:** C22H31BO3  
**SMILES:** CB1OC=C(C2CCC3C4CCC5=CC(=O)CCC5(C)C4CCC23C)O1  
**Mol. weight [g/mol]:** 354.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	5.141		Crippen Method
rinpol	2935.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525134&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  
**rinpol:** Non-polar retention indices

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