

# cannabidiolic acid, methyl-boronate

**Inchi:** InChI=1S/C23H31BO4/c1-6-7-8-9-16-13-19(25)21(22-20(16)23(26)28-24(5)27-22)18-12-2  
**InchiKey:** AUUHLCMQVONELA-MSOLQXFVSA-N  
**Formula:** C23H31BO4  
**SMILES:** C=C(C)C1CCC(C)=CC1c1c(O)cc(CCCCC)c2c1OB(C)OC2=O  
**Mol. weight [g/mol]:** 382.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	5.808		Crippen Method
rinpol	2595.00		NIST Webbook

## 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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487522&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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<https://www.chemeo.com/cid/11-273-6/cannabidiolic-acid-methyl-boronate.pdf>

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