

# Castasterone, methaneboronate

**Inchi:** InChI=1S/C30H50B2O5/c1-16(2)17(3)27-28(37-32(8)36-27)18(4)20-9-10-21-19-13-24(3)  
**InchiKey:** YDYBTAUNWYTXMW-MOWAKGPUSA-N  
**Formula:** C30H50B2O5  
**SMILES:** CB1OC2CC3C(=O)CC4C(CCC5(C)C(C(C)C6OB(C)OC6C(C)C(C)C)CCC45)C3(C)CC2O  
**Mol. weight [g/mol]:** 512.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	6.166		Crippen Method
rinpol	3618.00		NIST Webbook
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## 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=R497188&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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<https://www.chemeo.com/cid/43-557-6/Castasterone-methaneboronate.pdf>

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