

# 5-«alpha»-Pregnane-3-«beta»,17-«alpha»,20-«alpha»-triol methylboronate

InChI: InChI=1S/C22H37BO3/c1-14-22(26-23(4)25-14)12-9-19-17-6-5-15-13-16(24)7-10-20(15,16)/m1  
InChIKey: IVXGLDZOCJYIHH-JWGWEIGNSA-N  
Formula: C22H37BO3  
SMILES: CB1OC(C)C2(CCC3C4CCC5CC(O)CCC5(C)C4CCC32C)O1  
Mol. weight [g/mol]: 360.34

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -3.50   |      | Crippen Method |
| logp          | 4.682   |      | Crippen Method |
| rinpol        | 2705.00 |      | NIST Webbook   |
| rinpol        | 2705.00 |      | 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=R149943&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## Legend

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

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