

# 5-«alpha»-Pregnane-17-«alpha»,20-«alpha»-diol, methylboronate

InChI: InChI=1S/C22H37BO2/c1-15-22(25-23(4)24-15)14-11-19-17-9-8-16-7-5-6-12-20(16,2)18

InChIKey: ABMFHNLMTYOWJJN-OXHDMRKJSA-N

Formula: C<sub>22</sub>H<sub>37</sub>BO<sub>2</sub>

SMILES: CB1OC(C)C2(CCC3C4CCC5CCCCC5(C)C4CCC32C)O1

Mol. weight [g/mol]: 344.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	5.711		Crippen Method
rinpol	2455.00		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=R149750&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/35-921-0/5-alpha-Pregnane-17-alpha-20-alpha-diol-methylboronate.pdf>

Generated by Cheméo on 2024-05-09 19:21:51.524098582 +0000 UTC m=+17571760.444675895.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.