

5-«alpha»-Pregnane-17-«alpha»,20-«beta»-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-MMRAWNDHSA-N

Formula: C22H37BO2

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 | 2440.00 | | NIST Webbook |
| rinpol | 2440.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149849&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/19-158-6/5-alpha-Pregnane-17-alpha-20-beta-diol-methylboronate.pdf>

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