

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

InChI: InChI=1S/C23H39BO2/c1-15-23(14-24(4)26-15)12-9-20-18-6-5-16-13-17(25)7-10-21(16,17)/1-2
InchiKey: DMVOTGNHNNGULM-GLXUTGLSSA-N
Formula: C23H39BO2
SMILES: CB1CC2(CCC3C4CCC5CC(O)CCC5(C)C4CCC32C)C(C)O1
Mol. weight [g/mol]: 358.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	5.416		Crippen Method
rinpol	2585.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R485724&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/42-738-6/5-beta-pregnane-3-alpha-17-alpha-20-beta-triol-17-20-methylboronate.pdf>

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