

5-«alpha»-Pregnane-3-«beta»,17-«alpha»,20-«beta»-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-VDQIJORPSA-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	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149998&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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