

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

InChI: InChI=1S/C25H45BO3Si/c1-17-25(29-26(4)27-17)15-12-22-20-9-8-18-16-19(28-30(5,6)7)/m1
InChIKey: QPQREXPMPYCKSEL-AUPXAGJVSA-N
Formula: C25H45BO3Si
SMILES: CB1OC(C)C2(CCC3C4CCC5CC(O[Si](C)(C)C)CCC5(C)C4CCC32C)O1
Mol. weight [g/mol]: 432.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	6.541		Crippen Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R150002&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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<https://www.cheméo.com/cid/20-141-2/5-alpha-Pregnane-3-beta-17-alpha-20-beta-triol-methylboronate-TMS.pdf>

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