

5-«alpha»-Pregnane-17-«alpha»,20-«beta»,21-triol-methylboronate, TMS

InChI: InChI=1S/C25H45BO3Si/c1-23-14-8-7-9-18(23)10-11-19-20(23)12-15-24(2)21(19)13-16-25
InChIKey: IVIMADLWVLPJLL-PNIAWLBSA-N

Formula: C₂₅H₄₅BO₃Si

SMILES: CB1OCC(C2(O[Si](C)(C)C)CCC3C4CCC5CCCCC5(C)C4CCC32C)O1

Mol. weight [g/mol]: 432.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	6.543		Crippen Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		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=R149785&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/51-817-8/5-alpha-Pregnane-17-alpha-20-beta-21-triol-methylboronate-TMS.pdf>

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