

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

InChI: InChI=1S/C22H37BO3/c1-20-11-5-4-6-15(20)7-8-16-17(20)9-12-21(2)18(16)10-13-22(21)14-3
InChIKey: XNVCVOFXYDNYED-PUODDTFBSA-N

Formula: C22H37BO3
SMILES: CB1OCC(C2(O)CCC3C4CCC5CCCCC5(C)C4CCC32C)O1
Mol. weight [g/mol]: 360.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	4.684		Crippen Method
rinpol	2690.00		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=R149770&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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