

17«alpha»,20«beta»,21-Trihydroxypregn-4-en-3-one methylboronate

InChI: InChI=1S/C22H33BO4/c1-20-9-6-15(24)12-14(20)4-5-16-17(20)7-10-21(2)18(16)8-11-22
InChIKey: PQXGMOHODMJBLI-WARUMDEKSA-N

Formula: C22H33BO4

SMILES: CB1OCC(C2(O)CCC3C4CCC5=CC(=O)CCC5(C)C4CCC32C)O1

Mol. weight [g/mol]: 372.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	3.783		Crippen Method
rinpol	2970.00		NIST Webbook
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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=R525010&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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