

5-«alpha»-Pregnane-20-«beta»,21-diol, methylboronate

Inchi: InChI=1S/C22H37BO2/c1-21-12-5-4-6-15(21)7-8-16-17-9-10-19(20-14-24-23(3)25-20)22
InchiKey: QXLQOGXVJHVLBW-QYWJFSONSA-N
Formula: C22H37BO2
SMILES: CB1OCC(C2CCC3C4CCC5CCCCC5(C)C4CCC23C)O1
Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	5.569		Crippen Method
rinpol	2560.00		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=R149923&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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<https://www.chemeo.com/cid/53-553-9/5-alpha-Pregnane-20-beta-21-diol-methylboronate.pdf>

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