

5-Pregnene-3«beta»,20«beta»,21-triol, methylboronate

Inchi: InChI=1S/C22H35BO3/c1-21-10-8-15(24)12-14(21)4-5-16-17-6-7-19(20-13-25-23(3)26-2
InchiKey: RJHXJJQFJHVXNR-SAZUVXTJSA-N
Formula: C22H35BO3
SMILES: CB1OCC(C2CCC3C4CC=C5CC(O)CCC5(C)C4CCC23C)O1
Mol. weight [g/mol]: 358.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	4.460		Crippen Method
rinpol	2810.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528891&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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