5-«alpha»-Pregnane-17-«alpha»,20-«alpha»-diol, methylboronate

Inchi: InChI=1S/C22H37BO2/c1-15-22(25-23(4)24-15)14-11-19-17-9-8-16-7-5-6-12-20(16,2)18
InchiKey: ABMHNLMTYOWJJN-OXHDMRKJSA-N
Formula: C22H37BO2
SMILES: CB1OC(C)C2(CCC3C4CCC5CCCCC5(C)C4CCC32C)O1
Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	5.711		Crippen Method
rinpol	2455.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149750&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices