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

Inchi: InChI=1S/C25H43BO3Si/c1-24-13-11-18(29-30(4,5)6)15-17(24)7-8-19-20-9-10-22(23-16

InchiKey: DYSJFFIPZVHTFM-PMAAMSHJSA-N

Formula: C25H43BO3Si

SMILES: CB1OCC(C2CCC3C4CC=C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)O1

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Cheméo Relay (1.0)
logp	6.319		Crippen Method
rinpol	2895.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tf	393.01	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R528831&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point