3-epi-2-deoxybrassinolide, methaneboronate-TMS

Inchi: InChI=1S/C31H55BO5Si/c1-18(2)19(3)26-27(36-32(7)35-26)20(4)22-11-12-23-28-24(14-

InchiKey: HCTNSNKPGFPWKI-XAGGBZALSA-N

Formula: C31H55BO5Si

SMILES: CB1OC(C(C)C(C)C)C(C(C)C2CCC3C4OC(=O)C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C

Mol. weight [g/mol]: 546.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.211		Crippen Method
rinpol	3915.00		NIST Webbook
rinpol	3915.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R497153&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices