

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(14-15-16-17)/1-2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31
InchiKey: HCTNSNKPGFPWKI-MUCOPARLSA-N
Formula: C31H55BO5Si
SMILES: CB1OC(C(C)C(C)C)C(C(C)C2CCC3C4OC(=O)C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)C3
Mol. weight [g/mol]: 546.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.211		Crippen Method
rinpol	3756.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R497148&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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