

«xi»-Hydroxybrassinolide, methaneboronate-TMS

Inchi: InChI=1S/C32H56B2O7Si/c1-18(26-27(40-34(8)39-26)19(2)30(3,4)41-42(9,10)11)20-12-
InchiKey: IYHJSBNROXPRMF-BDGASRDSSA-N
Formula: C32H56B2O7Si
SMILES: CB1OC2CC3C(=O)OC4C(CCC5(C)C(C(C)C6OB(C)OC6C(C)C(C)(C)O[Si](C)(C)C)CCC
Mol. weight [g/mol]: 602.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	6.477		Crippen Method
rinpol	3783.00		NIST Webbook
rinpol	3783.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R497133&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-004-2/xi-Hydroxybrassinolide-methaneboronate-TMS.pdf>

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