Thromboxane B2, reduced, methaneboronate, bis-TMS

Inchi: InChI=1S/C27H53BO6Si2/c1-9-10-13-16-23-19-20-26(33-28(2)32-23)24(25(29)21-22-31

InchiKey: QNKWIDWCPGWMLM-ADKQGXPBSA-N

Formula: C27H53BO6Si2

SMILES: CCCCCC1C=CC(C(CC=CCCCC(=O)O[Si](C)(C)C)C(O)CCO[Si](C)(C)C)OB(C)O1

Mol. weight [g/mol]: 540.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	6.738		Crippen Method
rinpol	2770.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526553&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