

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-ADKQGXPSA-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

Latest version available from:

<https://www.chemeo.com/cid/35-729-4/Thromboxane-B2-reduced-methaneboronate-bis-TMS.pdf>

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