

Thromboxane B2, tris-TMS

Inchi: InChI=1S/C29H58O6Si3/c1-11-12-15-18-24(33-36(2,3)4)21-22-26-25(27(23-29(31)32-26
InchiKey: IPOAFSHHUOPOBE-IESNQNSOSA-N
Formula: C29H58O6Si3
SMILES: CCCCCC(C=CC1OC(O)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 587.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.81		Crippen Method
logp	7.781		Crippen Method
rinpol	2760.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R526588&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/67-733-4/Thromboxane-B2-tris-TMS.pdf>

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