

Thromboxane B2, MO-tris-TMS, major

Inchi: InChI=1S/C30H61NO6Si3/c1-12-13-16-19-26(35-38(3,4)5)22-23-28(32)27(29(24-25-31-32)26)30-33-34-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: JFDCRNMLAHRWNH-OOFCMHOJSA-N
Formula: C30H61NO6Si3
SMILES: CCCCCC(C=CC(O)C(CC=CCCC(=O)O[Si](C)(C)C)C(CC=NOC)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 616.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	8.057		Crippen Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		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=R526528&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/70-748-4/Thromboxane-B2-MO-tris-TMS-major.pdf>

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