

Thromboxane B2, MO-tris-TMS, minor

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
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	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R526533&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/47-812-8/Thromboxane-B2-MO-tris-TMS-minor.pdf>

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