

13,14-Dihydro-15-keto-TxB2, BO-TMS, isomer # 1

Inchi: InChI=1S/C33H67NO6Si3/c1-12-14-18-21-28(34-36-26-15-13-2)24-25-30-29(22-19-16-17)23-31-32-33
InchiKey: CCNTZPCJTQDOEV-QQFSFTCTSA-N
Formula: C33H67NO6Si3
SMILES: CCCCC(CCC1OC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC=CCCC(=O)O[Si](C)(C)C)N
Mol. weight [g/mol]: 658.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	9.817		Crippen Method
rinpol	3215.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580775&Units=SI>

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.cheméo.com/cid/70-563-9/13-14-Dihydro-15-keto-TxB2-BO-TMS-isomer-1.pdf>

Generated by Cheméo on 2024-04-29 09:45:40.74363408 +0000 UTC m=+16673189.664211393.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.