

13,14-Dihydro-15-keto-TxB2, EO-TMS

Inchi: InChI=1S/C31H63NO6Si3/c1-12-14-17-20-26(32-34-13-2)23-24-28-27(21-18-15-16-19-2
InchiKey: CTHGMJFCBCFABA-RJSUQQFGSA-N
Formula: C31H63NO6Si3
SMILES: CCCCCC(CCC1OC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)=N
Mol. weight [g/mol]: 630.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	9.037		Crippen Method
rinpol	2914.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580804&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/21-281-6/13-14-Dihydro-15-keto-TxB2-EO-TMS.pdf>

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