

# TxB2, MO-TMS

**Inchi:** InChI=1S/C33H69NO6Si4/c1-15-16-19-22-29(37-41(3,4)5)25-26-31(38-42(6,7)8)30(32(2  
**InchiKey:** DAWLFOGOHREZST-XQINBFFOSA-N  
**Formula:** C33H69NO6Si4  
**SMILES:** CCCCCC(C=CC(O[Si](C)(C)C)C(CG=CCCCC(=O)O[Si](C)(C)C)C(CC=NOC)O[Si](C)(C)  
**Mol. weight [g/mol]:** 688.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	9.916		Crippen Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582033&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/54-636-6/TxB2-MO-TMS.pdf>

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