

# TxB2, BO-TMS, isomer # 2

**Inchi:** InChI=1S/C36H75NO6Si4/c1-15-17-21-24-32(40-44(3,4)5)27-28-34(41-45(6,7)8)33(25-2  
**InchiKey:** ZDKNWZCKFHUROO-PYQFQSJFSA-N  
**Formula:** C36H75NO6Si4  
**SMILES:** CCCCCC(C=CC(O[Si](C)(C)C)C(CG=CCCCC(=O)O[Si](C)(C)C)C(CC=NOCCCC)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 730.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	11.087		Crippen Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582013&Units=SI>  
**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)

## 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/120-390-5/TxB2-BO-TMS-isomer-2.pdf>

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