

TxB2, BO-TMS, isomer # 1

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	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582008&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.chemeo.com/cid/119-022-5/TxB2-BO-TMS-isomer-1.pdf>

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