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(CC=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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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