

Thromboxane B2, tris-TBDMS

Inchi: InChI=1S/C38H76O6Si3/c1-17-18-21-24-30(42-45(11,12)36(2,3)4)27-28-32-31(33(29-35
InchiKey: XQRPEYGADDUWES-UCIIDGISSA-N
Formula: C38H76O6Si3
SMILES: CCCCCC(C=CC1OC(O)CC(O[Si](C)(C)C(C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C(C)(C)
Mol. weight [g/mol]: 713.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	11.292		Crippen Method
rinpol	3405.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R526573&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/43-789-9/Thromboxane-B2-tris-TBDMS.pdf>

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