

3«beta»,5«alpha»,6«beta»-trihydroxysitostanol, TMS

TMS

InChI=1S/C38H76O3Si3/c1-16-29(27(2)3)18-17-28(4)32-19-20-33-31-25-35(40-43(10,11

InchiKey: QAAUNGMSVBDVIK-MLJULTOTSA-N

Formula: C38H76O3Si3

SMILES: CCC(CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4(O[Si](C)(C)C)CC(O[Si](C)(C)C)CCC4(C)C

Mol. weight [g/mol]: 665.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	11.768		Crippen Method
rinpol	3520.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395329&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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