

# 3«beta»,5«alpha»,6«beta»-trihydroxycholestanol, TMS

**Other names:**

5A-Cholestan-3B,5A,6B-triol, TMS

Cholestane-3«beta»,5«alpha»,6«beta»-triol, TMS

3«beta»,5«alpha»,6«beta»-trihydroxy-cholestane, TMS

**Inchi:** InChI=1S/C36H72O3Si3/c1-26(2)16-15-17-27(3)30-18-19-31-29-24-33(38-41(9,10)11)36

**InchiKey:** DLTPOCOBKWOAHI-DVEXUQKZSA-N

**Formula:** C36H72O3Si3

**SMILES:** CC(C)CCCC(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]:** 637.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	11.132		Crippen Method
rmpol	3405.00		NIST Webbook
rmpol	3405.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R108551&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rmpol:** Non-polar retention indices

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