

5«beta»-cholestane, 3«alpha»,7«beta»-dihydroxy, TMS

Inchi: InChI=1S/C33H64O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-31-29(18-20-33(27,28)5)32
InchiKey: SABSXFHUKZVEMF-RWMRLYLSSA-N
Formula: C33H64O2Si2
SMILES: CC(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 549.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	10.158		Crippen Method
rinpol	3285.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493928&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

Latest version available from:

<https://www.chemeo.com/cid/35-015-6/5-beta-cholestane-3-alpha-7-beta-dihydroxy-TMS.pdf>

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