

5-Cholesten-3-«beta»,27-diol, TMS

Other names:	27-Hydroxycholesterol, TMS 5-Cholesten-3B(25R),26-diol, TMS 5-Cholesten-3-«beta»,26-diol, TMS 26-Hydroxycholesterol, di-TMS
Inchi:	InChI=1S/C33H62O2Si2/c1-24(23-34-36(5,6)7)12-11-13-25(2)29-16-17-30-28-15-14-26-
InchiKey:	XPOWNWJGSYYWLA-TZWGRJOJSA-N
Formula:	C33H62O2Si2
SMILES:	CC(CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)CO[Si](C)(C)C
Mol. weight [g/mol]:	547.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	10.079		Crippen Method
rinpol	3470.00		NIST Webbook
rinpol	3459.00		NIST Webbook
rinpol	3450.00		NIST Webbook
rinpol	3455.00		NIST Webbook
rinpol	3450.00		NIST Webbook
rinpol	3450.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R11791&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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