5-Cholesten-3-«beta»-ol-7-one, TMS

Other names: 3B-Hydroxy-5-cholesten-7-one, TMS
7-Ketocholesterol, TMS
7-Oxocholesterol, TMS
Inchi: InChI=1S/C33H60O2Si2/c1-23(2)13-12-14-24(3)27-15-16-28-31-29(18-20-33(27,28)5)32
InchiKey: GRQGMVRZMUHBDW-MMEKYXELSA-N
Formula: C33H60O2Si2
SMILES: CC(C)CCCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21
Mol. weight [g/mol]: 545.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	10.347		Crippen Method
rinpol	3389.00		NIST Webbook
rinpol	3370.00		NIST Webbook
rinpol	3375.00		NIST Webbook
rinpol	3370.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R18567&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

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