

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-MMEKYYXELSA-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/ci9903071>

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.cheméo.com/cid/10-693-1/5-Cholesten-3-beta-ol-7-one-TMS.pdf>

Generated by Cheméo on 2024-04-18 07:20:08.792508231 +0000 UTC m=+15714057.713085546.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.