

(20S)-5«alpha»-cholestan-3«beta»,20,25-triol, DMESI

Inchi: InChI=1S/C39H78O3Si3/c1-15-43(9,10)40-31-23-27-37(6)30(29-31)19-20-32-33-21-22-3
InchiKey: RYULBNZHCYKPOE-WZHXPICFSA-N
Formula: C39H78O3Si3
SMILES: CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CCC2(C)C3CCC2C(C)(CCCC(C)(C)O[Si](C)(C)CC
Mol. weight [g/mol]: 679.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	12.446		Crippen Method
rinpol	3804.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279628&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/63-949-9/20S-5-alpha-cholestan-3-beta-20-25-triol-DMESI.pdf>

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