

7«alpha»-hydroxy-3-oxo-4-chol-24-oate, TMS

Inchi: InChI=1S/C33H60O4Si3/c1-23(13-16-30(34)37-40(10,11)12)26-14-15-27-31-28(18-20-32)
InchiKey: GGQFXVAOBWRSTK-RILFYBJCSA-N
Formula: C33H60O4Si3
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C
Mol. weight [g/mol]: 605.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	9.535		Crippen Method
rinpol	3295.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R492594&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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