1-Methyl-6«alpha»,7«alpha»-dihydroxyestrone, TMS

InChI: InChI=1S/C31H56O4Si4/c1-21-19-22(32-36(3,4)5)20-24-27(21)23-17-18-31(2)25(15-16-
InChIKey: ANTMMWDLXLMSNB-OYWOUPIPSA-N
Formula: C31H56O4Si4
SMILES: Cc1cc(O[Si](C)(C)C)cc2c1C1CCC3(C)C(O[Si](C)(C)C)=CCC3C1C(O[Si](C)(C)C)C2O[Si
Mol. weight [g/mol]: 605.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	9.590		Crippen Method
rinpol	2744.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305163&Units=SI

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.chemeo.com/cid/38-589-7/1-Methyl-6-alpha-7-alpha-dihydroxyestrone-TMS.pdf
Generated by Cheméo on 2025-12-22 01:39:37.605073099 +0000 UTC m=+6115775.135113753.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.