

17«alpha»,20«beta»,21-Trihydroxypregn-4-en-3-one-3-MO, 17,20,21-tris-TMS

InChI: 1S/C31H59NO4Si3O1-29-18-15-24(32-33-3)21-23(29)13-14-25-26(29)16-19-30(29)17-20-21-22-23-24-25-26-27-28-29-30-31
InChIKey: VQKWGPZGEROFQY-CWZYCZMTSA-N
Formula: C31H59NO4Si3
SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C)C
Mol. weight [g/mol]: 594.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.613		Crippen Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R524988&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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