

5«beta»-Pregnan-3«alpha»,11«beta»,17«alpha»,21«alpha»-MO-TMS (11-OH)

InChIKey: SJJWISDCLSBKEO-DXEIOIHHFSA-N

Formula: C₃₀H₅₉NO₅Si₃

SMILES: CON=C(CO[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3C(O)C

Mol. weight [g/mol]: 598.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	7.274		Crippen Method
rinpol	3182.00		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=R523465&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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