

5-«beta»-Pregnan-3-«alpha»,20-«alpha»,21-triol,

MeTMS

InChI: InChI=1S/C30H60O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)31

InChIKey: PCDMVFRHMJMCFX-KPQWWESTSA-N

Formula: C30H60O3Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	8.937		Crippen Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393467&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/51-206-6/5-beta-Pregnan-3-alpha-20-alpha-21-triol-MeTMS.pdf>

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