

5-«alpha»-Pregnane-17-«alpha»,20-«beta»,21-triol-tris-TMS

InChI: InChI=1S/C30H60O3Si3/c1-28-19-13-12-14-23(28)15-16-24-25(28)17-20-29(2)26(24)18-27
InChIKey: XCHVDXCTEBATMT-KCVPSGEOSA-N
Formula: C30H60O3Si3
SMILES: CC12CCCCC1CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	9.081		Crippen Method
rinpol	2870.00		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=R149809&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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<https://www.chemeo.com/cid/63-477-3/5-alpha-Pregnane-17-alpha-20-beta-21-triol-tris-TMS.pdf>

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