

5-«alpha»-Pregnan-3,17,20-triol, MeTMS

Inchi: InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21
InchiKey: KFUWLVZCEDFJIK-OOORMZHRS-A-N
Formula: C30H60O3Si3
SMILES: CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	9.079		Crippen Method
rinpol	2907.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393303&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/10-774-1/5-alpha-Pregnan-3-17-20-triol-MeTMS.pdf>

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