

Pregnan-3,17,20-triol, TMS

Inchi: InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)24-13-14-25-28-26(16-18-30(24,25)3)29(2)1
InchiKey: ANLFUEQWODEQDA-IEMWFTOSSA-N
Formula: C30H60O3Si3
SMILES: CC(O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	2916.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499624&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/61-837-5/Pregnan-3-17-20-triol-TMS.pdf>

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