

5-Pregnen-3,16,17-triol-20-one, TMS

Inchi: InChI=1S/C30H56O4Si3/c1-21(31)30(34-37(10,11)12)27(33-36(7,8)9)20-26-24-14-13-22
InchiKey: YWGBQVAQLXARBX-CTVMMKJVSA-N
Formula: C30H56O4Si3
SMILES: CC(=O)C1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CC
Mol. weight [g/mol]: 565.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	8.179		Crippen Method
rinpol	2848.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394222&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/60-189-6/5-Pregnen-3-16-17-triol-20-one-TMS.pdf>

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