

Pregnan-20-one, 3,17,21-tris[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»)-

Other names: Tetrahydrodeoxycortisol enol-TMS

Inchi: InChI=1S/C30H58O4Si3/c1-28-17-14-23(33-36(6,7)8)20-22(28)12-13-24-25(28)15-18-29

InchiKey: WBAVMJWNTRESLJ-BTILRRONSA-N

Formula: C30H58O4Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(=O)CO[Si](C)(C)C

Mol. weight [g/mol]: 567.04

CAS: 57397-20-3

Physical Properties

Property code	Value	Unit	Source
logp	8.260		Crippen Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57397203&Units=SI>

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/117-205-4/Pregnan-20-one-3-17-21-tris-trimethylsilyl-oxy-3-alpha-5-beta.pdf>

Generated by Cheméo on 2026-07-30 12:31:19.022950219 +0000 UTC m=+6355.599313463.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.