

5-pregnene-3«beta»,16«alpha»,20«alpha»-triol,

Other names:

5-Pregnene-3«beta»,16«alpha»,20«alpha»-triol, EO-TMS

Inchi: InChI=1S/C30H58O3Si3/c1-21(31-34(4,5)6)28-27(33-36(10,11)12)20-26-24-14-13-22-19

InchiKey: MZONKYFRXIRMRD-NGHDTWNHSA-N

Formula: C30H58O3Si3

SMILES: CC(O[Si](C)(C)C)C1C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21

Mol. weight [g/mol]: 551.04

Physical Properties

Property code	Value	Unit	Source
logp	8.856		Crippen Method
rinpol	2977.00		NIST Webbook
rinpol	2981.00		NIST Webbook
rinpol	2978.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tf	393.98	K	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R488312&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

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