5-«beta»-Pregnan-3-«alpha»,11-«beta»,20-«beta»-TMS

InchI:	InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)25-15-16-26-24-14-13-22-19-23(32-35(7,8)9)
InchiKey:	NWGHCYXPXWBNLK-KDVUPINTSA-N
Formula:	C30H60O3Si3
SMILES:	CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]:	553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486950&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/30-070-0/5-beta-Pregnan-3-alpha-11-beta-20-beta-triol-TMS.pdf
Generated by Cheméo on 2024-10-12 05:41:47.61213955 +0000 UTC m=+3292570.249108808.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.