5-«beta»-Pregnan-3-«alpha»,16-«alpha»-diol-20-on MeTMS

Inchi:	InChI=1S/C27H50O3Si2/c1-18(28)25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5
InchiKey:	WEEZFJRNCVQVEU-HCDFPIGGSA-N
Formula:	C27H50O3Si2
SMILES:	CC(=O)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393452&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/70-019-3/5-beta-Pregnan-3-alpha-16-alpha-diol-20-one-MeTMS.pdf
Generated by Cheméo on 2024-04-29 07:27:02.134175402 +0000 UTC m=+16664871.054752717.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.