5-«alpha»-Pregnan-3-«alpha»-16-«alpha»-diol-20-one TMS

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-WYEAUNGNSA-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
logp	7.284		Crippen Method
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook
tf	405.45	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R499520&Units=SI

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

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

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