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

Inchi: InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)

InchiKey: PSZRAFDARWUCMW-LWSJOAPHSA-N

Formula: C27H52O2Si2

SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 464.87

Physical Properties

Property code	Value	Unit	Source
logp	8.105		Crippen Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tf	383.81	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393398&Units=SI

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

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