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

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	2820.00		NIST Webbook
rinpol	2839.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tf	374.21	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385030&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