20«alpha»-hydroxy-pregn-4-en-3-one, MO-TMS, syn

Inchi: InChI=1S/C25H43NO2Si/c1-17(28-29(5,6)7)21-10-11-22-20-9-8-18-16-19(26-27-4)12-14

InchiKey: ROBQPFGUYCNUGC-UWCRPIHPSA-N

Formula: C25H43NO2Si

SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1

Mol. weight [g/mol]: 417.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Cheméo Relay (1.0)
logp	6.808		Crippen Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tf	389.70	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395765&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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point