20.alpha.-hydroxy-pregn-4-en-3-one, MO-TMS, anti

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-JVMMJAHXSA-N

Formula: C25H43NO2Si

SMILES: CO/N=C1\C=C2CCC3C(CC[C@@]4(C)C3CC[C@@H]4[C@H](C)O[Si](C)(C)C)[C@@]2

Mol. weight [g/mol]: 417.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Cheméo Relay (1.0)
logp	6.808		Crippen Method
tf	410.19	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R395750

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):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

tf: Normal melting (fusion) point