6.alpha.-hydroxy-pregn-4-ene-3,20-dione, MO-TMS, anti

Inchi: InChI=1S/C26H44N2O3Si/c1-17(27-29-4)20-9-10-21-19-16-24(31-32(6,7)8)23-15-18(28-

InchiKey: KSJDSPOSKCPKOH-CZGAFLNLSA-N

Formula: C26H44N2O3Si

SMILES: CO/N=C1\C=C2[C@@H](O[Si](C)(C)C)CC3C(CC[C@@]4(C)C3CC[C@@H]4/C(C)=N/O

Mol. weight [g/mol]: 460.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Cheméo Relay (1.0)
logp	6.420		Crippen Method
tf	413.36	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R395814

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

tf: Normal melting (fusion) point