17.alpha.-Hydroxypregnenolone, MO-TMS

Inchi: InChI=1S/C28H51NO3Si2/c1-20(29-30-4)28(32-34(8,9)10)18-15-25-23-12-11-21-19-22(3
InchiKey: QYVPPKLFPCFKFT-ANLSKKRDSA-N
Formula: C28H51NO3Si2
SMILES: CO/N=C(\C)[C@@]1(O[Si](C)(C)C)CC[C@H]2[C@@H]3CC=C4C[C@@H](O[Si](C)(C)C
Mol. weight [g/mol]: 505.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Cheméo Relay (1.0)
logp	7.782		Crippen Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R512722

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient