

Pregn-5-en-20-one, 3,16-bis[(trimethylsilyl)oxy]-, O-methyloxime, (3«beta»,16«alpha»)-

Other names: 16«alpha»-Hydroxypregnenolone, MO-TMS

Inchi: InChI=1S/C28H51NO3Si2/c1-19(29-30-4)26-25(32-34(8,9)10)18-24-22-12-11-20-17-21(3

InchiKey: YBQIXFAIJNZVRV-DZZATQCDSA-N

Formula: C28H51NO3Si2

SMILES: CON=C(C)C1C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 505.88

CAS: 57305-31-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Cheméo Relay (1.0)
logp	7.638		Crippen Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305314&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/124-647-6/Pregn-5-en-20-one-3-16-bis-trimethylsilyl-oxy-O-methyloxime-3-beta-16-alpha>

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