

Pregnan-20-one, 3,11,21-tris[(trimethylsilyloxy)-5«beta»-Pregnan-20-one, 3«alpha»,11«beta»,21-tris(trimethylsilyloxy)-5B-Pregnan-3A,11B,21-triol-20-one, MO TMS

O-methyloxime, (3«alpha»,5«beta»,11«beta»)-

Inchi: InChI=1S/C31H61NO4Si3/c1-30-18-17-23(35-38(7,8)9)19-22(30)13-14-24-25-15-16-26(27-28)O1
InchiKey: LTUTXXUPIPZWMI-GUPMVVFRSA-N
Formula: C31H61NO4Si3
SMILES: CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 596.08
CAS: 32206-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3012.00		NIST Webbook
rinpol	3009.00		NIST Webbook
rinpol	2994.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3009.00		NIST Webbook
rinpol	2994.00		NIST Webbook
rinpol	3012.00		NIST Webbook
rinpol	2994.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C32206681&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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