

5-Pregnan-11-one, 3«alpha»,20«alpha»,21-trihydroxy, MO-TMS

Inchi: InChI=1S/C31H61NO4Si3/c1-30-18-17-23(35-38(7,8)9)19-22(30)13-14-24-25-15-16-26(30)
InchiKey: FTSXTAWUYPNQGL-XIGZSRCMSA-N
Formula: C31H61NO4Si3
SMILES: CON=C1CC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3
Mol. weight [g/mol]: 596.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3092.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527269&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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