

5«xi»-Pregnan-11-one, 1«xi»,3«xi»,20«xi»-trihydroxy, TMSO-TMS

Inchi: InChI=1S/C33H67NO4Si4/c1-23(35-39(4,5)6)27-18-19-28-26-17-16-24-20-25(36-40(7,8))
InchiKey: GZWDWHIBUILDJG-RIHQVDFKSA-N
Formula: C33H67NO4Si4
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4(C)C3C(=NO[S
Mol. weight [g/mol]: 654.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	9.753		Crippen Method
rinpol	3036.00		NIST Webbook
rinpol	3036.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527249&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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