

3A,11B,21-Trihydroxy-5A-pregnan-20-one, 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(27,28)29
InchiKey: LTUTXXUPIPZWMI-QLWZGCKESA-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

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3024.00		NIST Webbook
rinpol	3030.00		NIST Webbook
rinpol	3011.00		NIST Webbook
rinpol	3028.00		NIST Webbook
rinpol	3026.00		NIST Webbook
rinpol	3011.00		NIST Webbook
rinpol	3011.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97509&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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