

17«alpha»,21-Dihydroxypregn-4-en-3,20-dione,

bis-MO-21-TMS

InChI: InChI=1S/C26H44N2O4Si/c1-24-13-10-19(27-30-3)16-18(24)8-9-20-21(24)11-14-25(2)26
InChIKey: ZWQYGFFYGLCOFP-KMITYEAQSA-N
Formula: C26H44N2O4Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C(CO[Si](C)(C)C)=NOC)C2(C)CC1
Mol. weight [g/mol]: 476.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	5.537		Crippen Method
rinpol	3165.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525050&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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