

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

bis-MO-21-TMS(d9)

Inchi: C[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C
InchiKey: ZWQYGNFYGLCOFP-CNRRNCJVSA-N
Formula: C₂₆H₃₅D₉N₂O₄Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C(CO[Si](C)(C)C)=NOC)C2(C)CC1
Mol. weight [g/mol]: 485.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	5.537		Crippen Method
rinpol	3155.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525065&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

Latest version available from:

<https://www.chemeo.com/cid/42-377-7/17-alpha-21-Dihydroxypregn-4-en-3-20-dione-bis-MO-21-TMS-d9.pdf>

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