

5«beta»-Pregnan-3«alpha»,17«alpha»,20«beta»-triol-3-(acetoxymethyl)silyl-17,20-dimethylsilylene

InChI: CC(=O)O[Si](C)(C)OC1CCC2C(CCC3C2CCC2(C)C3CCC23O[Si](C)(C)OC3C)C1
InChIKey: IAOSJGLYNDTDHW-VNXXHJGSXSA-N
Formula: C₂₆H₄₆O₅Si₂
SMILES: CC(=O)O[Si](C)(C)OC1CCC2C(CCC3C2CCC2(C)C3CCC23O[Si](C)(C)OC3C)C1
Mol. weight [g/mol]: 494.81

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.46 | | Crippen Method |
| logp | 6.165 | | Crippen Method |
| rinpol | 2885.00 | | 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=R525169&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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