5A-Estran-3B,17B-diol, 17A-ethyl, bis-TMS

Inchi: InChI=1S/C26H50O2Si2/c1-9-26(28-30(6,7)8)17-15-24-23-12-10-19-18-20(27-29(3,4)5)1
InchiKey: ASVCLJYMXYOOEI-XQNJYVOISA-N
Formula: C26H50O2Si2
SMILES: CCC1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 450.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.859		Crippen Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R92278&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices