6«alpha»-Hydroxy-4-Chloro-1,2,dehydro-17«alpha bis-TMS

Inchi: InChI=1S/C26H43ClO3Si2/c1-24-13-12-20(28)23(27)22(24)21(29-31(4,5)6)16-17-18(24)

InchiKey: TYFGLBZGTXUKIU-MBTZSFDLSA-N

Formula: C26H43ClO3Si2

SMILES: CC12C=CC(=O)C(Cl)=C1C(O[Si](C)(C)C)CC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]: 495.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	7.301		Crippen Method
rinpol	3139.00		NIST Webbook
rinpol	3139.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R262987&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