3,18-Dioxo-11«beta»,17«alpha»-dihydroxy-4-etien
acid, 20,18-lactone, 18,11-hemiacetal, MO-TMS

Inchi: InChI=1S/C24H35NO5Si/c1-22-10-8-15(25-27-2)12-14(22)6-7-16-17-9-11-24(30-31(3,4)5
InchiKey: LQJQOUIZYIXVAJ-BSDYKZPCSA-N
Formula: C24H35NO5Si
SMILES: CON=C1C=C2CCC3C(C4CC56C(OC(=O)C5(O[Si](C)(C)C)CCC36)O4)C2(C)CC1
Mol. weight [g/mol]: 445.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.414		Crippen Method
rinpol	3188.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R531872&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:
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