

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

Inchi: C24H35NO5Si
InchiKey: LQJQOUIZYTXVAJ-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

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=R531872&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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