GA95(1,2-didehydroGA20) isolactone, MeTMS

Inchi: InChI=1S/C23H32O5Si/c1-14-12-21-13-22(14,28-29(4,5)6)11-8-15(21)23-10-7-9-20(2,19
InchiKey: CWTLMASHPLNKBZ-HHBZDXFNSA-N
Formula: C23H32O5Si
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=CCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.004		Crippen Method
rinpol	2505.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2501.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R266023&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