GA25, 12-«alpha»-OH, Me-TMS

Inchi: InChI=1S/C28H46O7Si2/c1-17-15-27-16-18(17)19(34-36(5,6)7)14-20(27)28(25(31)35-37
InchiKey: MLBRZABYFWVKEL-OGMVWFAASA-N
Formula: C28H46O7Si2
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)O[Si](C)(C)C)CCCC(C)(C(=O)OC)C1C3C(
Mol. weight [g/mol]: 550.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	5.326		Crippen Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536991&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