ent-6«alpha»,7«alpha»-Dihydroxy trachylobanic acid, Me-TMS

Inchi: InChI=1S/C27H48O4Si2/c1-24-12-11-13-25(2,23(28)29-4)21(24)20(30-32(5,6)7)22(31-33

InchiKey: RNTLIJIWMLSSHA-UZIUJYAZSA-N

Formula: C27H48O4Si2

SMILES: COC(=O)C1(C)CCCC2(C)C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C13CC4C(CC21)C4(C)C3

Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	6.478		Crippen Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R559112&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