ent-6«alpha»,7«alpha»-(OH)2 KA, MeTMS

Inchi: InChI=1S/C27H48O4Si2/c1-18-16-27-17-19(18)12-13-20(27)25(2)14-11-15-26(3,24(28)2
InchiKey: CKTNFGJOVXLXMW-CMXDAODCSA-N
Formula: C27H48O4Si2
SMILES: C=C1CC23CC1CCC2C1(C)CCCC(C)(C(=O)OC)C1C(O[Si](C)(C)C)C3O[Si](C)(C)C
Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
logp	6.788		Crippen Method
rinpol	2582.00		NIST Webbook
rinpol	2581.00		NIST Webbook
rinpol	2588.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2593.00		NIST Webbook
rinpol	2581.00		NIST Webbook
rinpol	2593.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from: