Silane, [[(15«alpha»,16«alpha»,17«beta»)-estra-1,3,5(10)-t

Other names: Silane, [[(15«alpha»,16«alpha»,17«beta»)-estra-1,3,5(10)-triene-3,15,16,17-tetrayl]tetrakis(oxy)]t
15«alpha»-Hydroxyestriol, TMS

Inchi: InChI=1S/C30H56O4Si4/c1-30-19-18-24-23-17-15-22(31-35(2,3)4)20-21(23)14-16-25(24

InchiKey: RSQDODOMVGFYEA-SSAJSDKISA-N

Formula: C30H56O4Si4

SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(

Mol. weight [g/mol]: 593.11

CAS: 57305-24-5

Physical Properties

Property code	Value	Unit	Source
ie	8.34	eV	Cheméo Relay (1.0)
logp	8.636		Crippen Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
rinpol	3096.00		NIST Webbook
tf	362.88	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305245&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):

Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

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