

17-epi-Oxamesterone, per-TMS

Inchi: InChI=1S/C29H54O3Si3/c1-27-18-17-25(30-33(4,5)6)26(31-34(7,8)9)24(27)14-13-21-22
InchiKey: ABKPFKCGRAVRBX-ANDYGHRESA-N
Formula: C29H54O3Si3
SMILES: CC12CC=C(O[Si](C)(C)C)C(O[Si](C)(C)C)=C1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 534.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	9.084		Crippen Method
rinpol	2865.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R257915&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

Latest version available from:

<https://www.chemeo.com/cid/18-609-6/17-epi-Oxamesterone-per-TMS.pdf>

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