

Androst-1,4-dien-2z-hydroxymethyl-17«alpha»-methyl-17-TMS

InChIKey:

InChI=1S/C33H61ClO4Si4/c1-31-20-23(22-35-39(4,5)6)30(37-41(10,11)12)29(34)26(31)

Formula:

C33H61ClO4Si4

SMILES:

CC12C=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)=C(Cl)C1=CCC1C2C(O[Si](C)(C)C)CC2(C)C1

Mol. weight [g/mol]:

669.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	10.299		Crippen Method
rinpol	3096.00		NIST Webbook
rinpol	3027.00		NIST Webbook
rinpol	3096.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R322019&Units=SI>

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.cheméo.com/cid/48-594-0/Androst-1-4-dien-2z-hydroxymethyl-17-alpha-methyl-11-alpha-17-beta-diol-3->

Generated by Cheméo on 2025-12-19 14:18:30.025423734 +0000 UTC m=+5902107.555464389.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.