

17-«beta»-Hydroxy-17-«alpha»-methyl-5-«beta»-androst-1-en-3-one-per-TMS

InChI: InChI=1S/C26H46O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InChIKey: LBFJZCFDESSUPM-SJNQKHIZSA-N
Formula: C26H46O2Si2
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 446.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	7.761		Crippen Method
rinpol	2570.00		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=R257371&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/40-565-0/17-beta-Hydroxy-17-alpha-methyl-5-beta-androst-1-en-3-one-per-TMS.pdf>

Generated by Cheméo on 2024-02-28 05:17:05.201122175 +0000 UTC m=+11386674.121699490.

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