

17-«beta»-Methyl-5-«beta»-androst-1-ene-3-«alpha»-diol-per-TMS

InChI: InChI=1S/C26H48O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InChIKey: FKXKDLQNCNDLSD-PLXSYBJCSA-N
Formula: C26H48O2Si2
SMILES: CC12C=CC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 448.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	7.635		Crippen Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R257524&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/64-640-0/17-beta-Methyl-5-beta-androst-1-ene-3-alpha-17-alpha-diol-per-TMS.pdf>

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