

17-«beta»-Methyl-5-«alpha»-androstan-3-«alpha»,

per-TMS
InChI: 1S/C26H50O2Si2/c1-24-15-12-20(27-29(4,5)6)18-19(24)10-11-21-22(24)13-16-25
InChIKey: GNQZRHQPXWSWJC-JNAXAXHOSA-N

Formula:

C26H50O2Si2

SMILES:

CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]:

450.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.859		Crippen Method
rinpol	2482.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R257460&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.chemeo.com/cid/15-402-8/17-beta-Methyl-5-alpha-androstan-3-alpha-17-alpha-diol-per-TMS.pdf>

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