

5«beta»-Androstan-3«alpha»,11«beta»-diol-17-one (Androsterone), MO-3,11-bis-TMS

InChI: InChI=1S/C26H49NO3Si2(c1-25-15-14-13-21-11(2,5)6)16-18(25)10-11-20-21-12-13-23(24)26)O1
InChIKey: XCNGMXXKDGICALRD-CBBXMSQWSA-N

Formula: C₂₆H₄₉NO₃Si₂

SMILES: CON=C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	7.082		Crippen Method
rinpol	2712.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523381&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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