2-keto,3-methyl-5«alpha»-androstan-17«beta»-ol, monoTBDMS

Inchi: InChI=1S/C26H46O2Si/c1-17-15-18-9-10-19-20-11-12-23(28-29(7,8)24(2,3)4)25(20,5)14

InchiKey: PYOFJWYFMHWUPH-AZEQZINBSA-N

Formula: C26H46O2Si

SMILES: CC1CC2CCC3C(CCC4(C)C(O[Si](C)(C)C(C)(C)C)CCC34)C2(C)CC1=O

Mol. weight [g/mol]: 418.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	7.235		Crippen Method
rinpol	2849.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385901&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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/69-084-3/2-keto-3-methyl-5-alpha-androstan-17-beta-ol-monoTBDMS.pdf
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