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

Inchi: InChI=1S/C23H40O2Si/c1-15-13-16-7-8-17-18-9-10-21(25-26(4,5)6)22(18,2)12-11-19(17

InchiKey: CEAVWRRRPOYXDW-HGGFXEPUSA-N

Formula: C23H40O2Si

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

Mol. weight [g/mol]: 376.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	6.064		Crippen Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385916&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