5«beta»-Androst-1-ene-3,17-dione, mono-TMS

Inchi: InChI=1S/C22H34O2Si/c1-21-12-10-16(24-25(3,4)5)14-15(21)6-7-17-18-8-9-20(23)22(18

InchiKey: MMIMIPWPVFQIMX-YFJQCNEPSA-N

Formula: C22H34O2Si

SMILES: CC12CCC3C(CCC4C=C(O[Si](C)(C)C)C=CC43C)C1CCC2=O

Mol. weight [g/mol]: 358.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	5.720		Crippen Method
rinpol	2452.00		NIST Webbook
rinpol	2468.00		NIST Webbook
rinpol	2452.00		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=R494674&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices