Androstane-11,17-dione, 3-[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»)-

Other names: 5«beta»-Androstane-11,17-dione, 3«alpha»-(trimethylsiloxy)-
3-[(Trimethylsilyl)oxy]androstane-11,17-dione-, (3«alpha»,5«beta»)-
11-Ketoetiocholanolone TMS
11-Ketoetiocholanolone, tms derivative

Inchi: InChI=1S/C22H36O3Si/c1-21-11-10-15(25-26(3,4)5)12-14(21)6-7-16-17-8-9-19(24)22(17

InchiKey: CCJDJZHCDREQKR-UHFFFAOYSA-N

Formula: C22H36O3Si

SMILES: CC12CC(=O)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 376.60

CAS: 5042-90-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	4.997		Crippen Method
rinpol	2622.00		NIST Webbook
rinpol	2611.00		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=C5042900&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices