5-«alpha»-Androstan-3-«beta»-ol-17-«beta»-carbo MeTMS

Inchi: InChI=1S/C24H42O3Si/c1-23-13-11-17(27-28(4,5)6)15-16(23)7-8-18-19-9-10-21(22(25)2

InchiKey: WGNHKXCUYIUHGD-HEFXAHKCSA-N

Formula: C24H42O3Si

SMILES: COC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 406.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	6.038		Crippen Method
rinpol	2720.00		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=R393294&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices