Aetiocholanolone, MO-TBDMS

Inchi: InChI=1S/C26H47NO2Si/c1-24(2,3)30(7,8)29-19-13-15-25(4)18(17-19)9-10-20-21-11-12
InchiKey: ATAVHXFPXLCEHX-YAWSDBHMSA-N
Formula: C26H47NO2Si
SMILES: CON=C1CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 433.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	7.422		Crippen Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R594373&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