Etiocholanolone, MO TMS

Inchi: InChI=1S/C23H41NO2Si/c1-22-13-11-17(26-27(4,5)6)15-16(22)7-8-18-19-9-10-21(24-25
InchiKey: OQODXBKTVOKPMR-PNLBLRPCSA-N
Formula: C23H41NO2Si
SMILES: CON=C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 391.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	6.252		Crippen Method
rinpol	2554.00		NIST Webbook
rinpol	2575.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2539.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2544.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2568.00		NIST Webbook
rinpol	2579.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2568.00		NIST Webbook
rinpol	2504.00		NIST Webbook
rinpol	2492.00		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=R92698&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices