Androstenedione (Androst-4-en-3,17-dione), TMS

Inchi: InChI=1S/C25H42O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: NZWSFMJGXZUTCA-GGAKRVASSA-N

Formula: C25H42O2Si2

SMILES: CC12CC=C(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12

Mol. weight [g/mol]: 430.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	7.640		Crippen Method
rinpol	2678.00		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=R585478&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

https://www.chemeo.com/cid/10-101-7/Androstenedione-Androst-4-en-3-17-dione-TMS.pdf

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