

5«beta»-Androst-1-ene-3,17-dione, mono-TMS

Inchi: InChI=1S/C22H34O2Si/c1-21-12-10-16(24-25(3,4)5)14-15(21)6-7-17-18-8-9-20(23)22(18)
InchiKey: MMIMIPWPVFQIMX-YFJQCNEPSA-N
Formula: C₂₂H₃₄O₂Si
SMILES: CC12CCC3C(CCC4C=C(O[Si](C)(C)C)C=CC43C)C1CCC2=O
Mol. weight [g/mol]: 358.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	5.720		Crippen Method
rinpol	2452.00		NIST Webbook
rinpol	2468.00		NIST Webbook
rinpol	2452.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R494674&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.cheméo.com/cid/56-164-8/5-beta-Androst-1-ene-3-17-dione-mono-TMS.pdf>

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