

4,16-Androstadien-3-one, TMS

Inchi: InChI=1S/C22H34OSi/c1-21-12-6-7-19(21)18-9-8-16-15-17(23-24(3,4)5)10-14-22(16,2)2
InchiKey: UIEAIMWJTJUB-WAYZNYOTSA-N
Formula: C₂₂H₃₄OSi
SMILES: CC12C=CCC1C1CCC3=CC(O[Si](C)(C)C)=CCC3(C)C1CC2
Mol. weight [g/mol]: 342.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.60		Crippen Method
logp	6.461		Crippen Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149636&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/37-672-5/4-16-Androstadien-3-one-TMS.pdf>

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