

Ergosta-5,7,9(11),22-tetraen-3«beta»-ol, TMS

Inchi: InChI=1S/C31H50OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7)
InchiKey: VIAWZTXJCLSWAW-SSOLSQPGSA-N
Formula: C31H50OSi
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=CC=C4CC(O[Si](C)(C)C)CCC4(C)C3=CCC21C
Mol. weight [g/mol]: 466.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.35		Crippen Method
logp	9.110		Crippen Method
rinpol	3161.00		NIST Webbook
rinpol	3161.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273026&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/50-920-4/Ergosta-5-7-9-11-22-tetraen-3-beta-ol-TMS.pdf>

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