

Androst-5,9(11)-diene-3-«beta»,17-«beta»-diol, TMS

Inchi: InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-28)/h1-10,12-14,16,18,20-22,24-25,27-28H,23H2,26H3
InchiKey: GUZYQHLPCCWDQG-SUQRNSRXSA-N
Formula: C25H44O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2=CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	7.309		Crippen Method
rinpol	2618.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2618.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385387&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/40-048-4/Androst-5-9-11-diene-3-beta-17-beta-diol-TMS.pdf>

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