

17«alpha»-hydroxy-5«alpha»-androstan-3-one (2-enol), per-TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: QXTVKDCDCWLKJJ-STHJLMPXSA-N
Formula: C25H46O2Si2
SMILES: CC12CC=C(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	7.594		Crippen Method
rinpol	2569.00		NIST Webbook
rinpol	2644.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R518339&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/24-409-1/17-alpha-hydroxy-5-alpha-androstan-3-one-2-enol-per-TMS.pdf>

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