

6«beta»-Hydroxy-Testosterone, bis-TMS

Inchi: InChI=1S/C25H44O3Si2/c1-24-13-11-17(26)15-21(24)22(27-29(3,4)5)16-18-19-9-10-23(24)
InchiKey: WPOAKICUPRIZOL-FWHLWJSISA-N
Formula: C₂₅H₄₄O₃Si₂
SMILES: CC12CCC(=O)C=C1C(O[Si](C)(C)C)CC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 448.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	6.568		Crippen Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263133&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/36-110-9/6-beta-Hydroxy-Testosterone-bis-TMS.pdf>

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