

5B-Estran-3-on-17B-ol, 17A-methyl, TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-21-20-12-10-19(26-28(3,4)5)17-18(20)9-11-22(21)
InchiKey: MPZYQHGBNUETKH-QGBUBSOZSA-N
Formula: C25H46O2Si2
SMILES: CC1(O[Si](C)(C)C)CCC2C3CCC4C=C(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	7.594		Crippen Method
rinpol	2550.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92424&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/64-111-7/5B-Estran-3-on-17B-ol-17A-methyl-TMS.pdf>

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