

Estran-4-on-17B-ol, 17A-methyl, TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-16-14-19-18-10-9-11-23(26-28(3,4)5)21(18)13-12-20(19)
InchiKey: XWMOVJSLBZPALE-FDKWZYQFSA-N
Formula: C25H46O2Si2
SMILES: CC1(O[Si](C)(C)C)CCC2C3CCC4=C(O[Si](C)(C)C)CCCC4C3CCC21C
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.739		Crippen Method
rinpol	2660.00		NIST Webbook
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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=R92474&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/63-399-0/Estran-4-on-17B-ol-17A-methyl-TMS.pdf>

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