

5A-Estran-3A,17B-diol, 17A-ethyl, bis-TMS

Inchi: InChI=1S/C26H50O2Si2/c1-9-26(28-30(6,7)8)17-15-24-23-12-10-19-18-20(27-29(3,4)5)1
InchiKey: ASVCLJYMXYOOEI-HHVFTYGKSA-N
Formula: C₂₆H₅₀O₂Si₂
SMILES: CCC1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 450.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	7.859		Crippen Method
rinpol	2660.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2660.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92189&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/49-817-1/5A-Estran-3A-17B-diol-17A-ethyl-bis-TMS.pdf>

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