

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

Inchi: InChI=1S/C26H48O2Si2/c1-9-26(28-30(6,7)8)17-15-24-23-12-10-19-18-20(27-29(3,4)5)1
InchiKey: ISGBJAVXHCXBMH-BKNKQISA-N
Formula: C₂₆H₄₈O₂Si₂
SMILES: CCC1(O[Si](C)(C)C)CCC2C3CCC4C=C(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 448.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	7.985		Crippen Method
rinpol	2670.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92410&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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