

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

Inchi: InChI=1S/C24H44O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey: DUKROBATFNHXPR-FFCTVPSNSA-N
Formula: C24H44O2Si2
SMILES: CC12CCC3C4CCC(O[Si](C)(C)C)=CC4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 420.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	7.204		Crippen Method
rinpol	2470.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92438&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/26-994-0/5B-Estran-3-on-17B-ol-TMS.pdf>

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