

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

Inchi: InChI=1S/C25H48O2Si2/c1-24-15-13-21-20-12-10-19(26-28(3,4)5)17-18(20)9-11-22(21)
InchiKey: JJEJKZMOLJFLPC-XZZKANODSA-N
Formula: C25H48O2Si2
SMILES: CC1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 436.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	7.469		Crippen Method
rinpol	2545.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2545.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92193&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/45-200-9/5A-Estran-3A-17B-diol-17A-methyl-bis-TMS.pdf>

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