

Estriol. VDMS

Inchi: InChI=1S/C29H48O3Si3/c1-11-34(7,8)30-22-14-16-23-21(19-22)13-15-25-24(23)17-18-2
InchiKey: XQHZGBFFRKDFRB-KLUNGUGNSA-N
Formula: C29H48O3Si3
SMILES: C=C[Si](C)(C)Oc1ccc2c(c1)CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C=C
Mol. weight [g/mol]: 528.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	7.997		Crippen Method
rinpol	3170.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529572&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/23-549-7/Estriol-VDMS.pdf>

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