5-Pregnen-3«beta»,20«alpha»-diol, allyl-DMS

Inchi: InChI=1S/C31H54O2Si2/c1-10-20-34(6,7)32-23(3)27-14-15-28-26-13-12-24-22-25(33-35
InchiKey: ZDYBOLVXBJVBKH-FDYVNFRISA-N
Formula: C31H54O2Si2
SMILES: C=CC[Si](C)(C)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)O[Si](C)(C)CC=C)CCC32)C1
Mol. weight [g/mol]: 514.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.99		Crippen Method
logp	9.138		Crippen Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526251&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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