

Pregn-5-en-20-one, 3-[(dimethyl-2-propenylsilyl)oxy]-, (3«beta»)-

Other names:

3«beta»-allyldimethylsilyloxy pregn-5-en-20-one

5-Pregnen-3«beta»-ol-20-one, allyl-DMS

Inchi: InChI=1S/C26H42O2Si/c1-7-16-29(5,6)28-20-12-14-25(3)19(17-20)8-9-21-23-11-10-22(1)

InchiKey: OEPZKUFNKBWSOF-NWZRQPDOSA-N

Formula: C26H42O2Si

SMILES: C=CC[Si](C)(C)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1

Mol. weight [g/mol]: 414.70

CAS: 61727-39-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	6.931		Crippen Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook

Sources

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C61727397&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

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