

5-Pregnen-3«beta»-ol-20-one, VDMS

Inchi: InChI=1S/C25H40O2Si/c1-7-28(5,6)27-19-12-14-24(3)18(16-19)8-9-20-22-11-10-21(17(2
InchiKey: IXUFWZYALROGLB-SZGGNGORSA-N
Formula: C25H40O2Si
SMILES: C=C[Si](C)(C)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
Mol. weight [g/mol]: 400.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	6.470		Crippen Method
rinpol	2813.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529552&Units=SI>

Legend

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

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