

Pregnan-2,3-diol-20-one, TMS

Inchi: InChI=1S/C27H48O3Si2/c1-18(28)21-12-13-22-20-11-10-19-16-24(29-31(4,5)6)25(30-32)
InchiKey: WPHLIUDJYNPPGD-CEPRCQELSA-N
Formula: C27H48O3Si2
SMILES: CC(=O)C1CCC2C3CC=C4CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC4(C)C3CCC12C
Mol. weight [g/mol]: 476.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	7.205		Crippen Method
rinpol	2804.00		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=R394420&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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