

20«beta»,21-Dihydroxypregn-4-en-3-one, 20,21-bis-TMS

Inchi: InChI=1S/C27H48O3Si2/c1-26-15-13-20(28)17-19(26)9-10-21-22-11-12-24(27(22,2)16-1
InchiKey: PKWNPIGWBFISPD-ACEMGPOESA-N
Formula: C27H48O3Si2
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 476.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	7.206		Crippen Method
rinsol	3095.00		NIST Webbook
rinsol	3095.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525114&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/26-843-7/20-beta-21-Dihydroxypregn-4-en-3-one-20-21-bis-TMS.pdf>

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