

*5«beta»-Pregnane-3«alpha», 20«beta»-diol-11-one, MO TMS

Inchi: InChI=1S/C26H49NO3Si2/c1-17(29-31(3,4)5)20-13-14-22-23-11-9-18-15-19(30-32(6,7)8)
InchiKey: MOUGWOFPPKPNTL-WIKYTUNOSA-N
Formula: C26H49NO3Si2
SMILES: CON=C1CC2C(C(C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3C12
Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	6.938		Crippen Method
rinpol	2886.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R250281&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-009-6/5-beta-Pregnane-3-alpha-20-beta-diol-11-one-MO-TMS.pdf>

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