

5«beta»-Pregnane-20-one-3«alpha»,21-diol, EO-TMS, # 1

Inchi: InChI=1S/C28H53NO3Si2/c1-9-30-29-27(19-31-33(3,4)5)26-15-14-25-24-12-10-20-18-21
InchiKey: KJZKGCMYIBJAAZ-HAEBBLMHSA-N
Formula: C28H53NO3Si2
SMILES: CCON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC12C
Mol. weight [g/mol]: 507.90

Physical Properties

Property code	Value	Unit	Source
logp	7.719		Crippen Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527061&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

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