

5«beta»-Pregnane-3«alpha»,20«alpha»-diol, EO-TMS

Inchi: InChI=1S/C26H50O2Si2/c1-18(27-29(3,4)5)24-13-14-25-23-11-9-19-17-20(28-30(6,7)8)1
InchiKey: ZIOHXUGXOHHKHG-VODVBZFSVSA-N
Formula: C₂₆H₅₀O₂Si₂
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC12C
Mol. weight [g/mol]: 450.85

Physical Properties

Property code	Value	Unit	Source
logp	7.715		Crippen Method
rinpol	2771.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2771.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527209&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/114-956-4/5-beta-Pregnane-3-alpha-20-alpha-diol-EO-TMS.pdf>

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