

5«beta»-Pregnan-3«alpha»,11«beta»,17«alpha»,21«alpha»-MO-tetrakis-TMS

Inchi: C33H67NO5Si4/c1-32-22-29(38-42(9,10)11)31-26-18-16-25(37-41(6,7)8)21-24
InchiKey: HPHPNLQTTJNNGK-FZHUUYIDSA-N
Formula: C33H67NO5Si4
SMILES: CON=C(CO[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4C3C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 670.23

Physical Properties

Property code	Value	Unit	Source
logp	9.133		Crippen Method
rinpol	3179.00		NIST Webbook
rinpol	3179.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523450&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/116-315-3/5-beta-Pregnan-3-alpha-11-beta-17-alpha-21-tetrol-20-one-MO-tetrakis-TMS>

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