

5-«beta»-Pregnan-3-«alpha»,16-«alpha»-diol-20-one

MeTMS

InChI: InChI=1S/C27H50O3Si2/c1-18(28)25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5)6)33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-18,25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5)6)33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/t1-18,25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5)6)33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/m-1/s-1

InChIKey:

WEEZFJRNCVQVEU-HCDFPIGGSA-N

Formula:

C₂₇H₅₀O₃Si₂

SMILES:

CC(=O)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]:

478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R393452&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/70-019-3/5-beta-Pregnan-3-alpha-16-alpha-diol-20-one-MeTMS.pdf>

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