

5-Pregnen-3-«alpha»,20-«alpha»-diol-20-GlcNAc

TMS

InchiKey:

InChI=1S/C41H79NO7Si4/c1-27(32-19-20-33-31-18-17-29-25-30(47-51(8,9)10)21-23-40

IHXNCGCWSBPANW-IVIGLZASSA-N

Formula:

C41H79NO7Si4

SMILES:

CC(=O)NC1C(OC(C)C2CCC3C4CC=C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)OC(CO[

Mol. weight [g/mol]:

810.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.83 | | Crippen Method |
| logp | 9.712 | | Crippen Method |
| rinpol | 4383.00 | | NIST Webbook |

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R394237&Units=SI>

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.cheméo.com/cid/36-761-7/5-Pregnen-3-alpha-20-alpha-diol-20-GlcNAc-TMS.pdf>

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