

21-Hydroxypregn-4-en-3,20-dione, bis-MO-21-TMS

Inchi: InChI=1S/C26H44N2O3Si/c1-25-14-12-19(27-29-3)16-18(25)8-9-20-21-10-11-23(26(21,22)17)24
InchiKey: QDEFZWVWFGZSRJ-WQYHOECPSA-N
Formula: C₂₆H₄₄N₂O₃Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(CO[Si](C)(C)C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	6.422		Crippen Method
rinpol	3030.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525149&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/33-052-7/21-Hydroxypregn-4-en-3-20-dione-bis-MO-21-TMS.pdf>

Generated by Cheméo on 2024-05-02 18:15:15.439134864 +0000 UTC m=+16962964.359712180.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.