

6«beta»-hydroxy-pregn-4-ene-3,20-dione, MO-TMS, syn

Inchi: InChI=1S/C26H44N2O3Si/c1-17(27-29-4)20-9-10-21-19-16-24(31-32(6,7)8)23-15-18(28-3)
InchiKey: KSJDSPOSKCPKOH-LXRDFICJSA-N
Formula: C26H44N2O3Si
SMILES: CON=C1C=C2C(O[Si](C)(C)C)CC3C(CCC4(C)C(C(C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Cheméo Relay (1.0)
logp	6.420		Crippen Method
rinpol	2923.00		NIST Webbook
rinpol	2923.00		NIST Webbook
tf	395.80	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395849&Units=SI>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/119-503-1/6-beta-hydroxy-pregn-4-ene-3-20-dione-MO-TMS-syn.pdf>

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