

5-«beta»-Pregnan-3-«beta»-ol-11-one, MO-TMS

Inchi: InChI=1S/C25H45NO2Si/c1-8-17-10-12-21-20-11-9-18-15-19(28-29(5,6)7)13-14-24(18,2
InchiKey: IFKSNQUFNAHUPS-GJWVOQCVSA-N
Formula: C25H45NO2Si
SMILES: CCC1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2563.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487111&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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/11-774-0/5-beta-Pregnan-3-beta-ol-11-one-MO-TMS.pdf>

Generated by Cheméo on 2024-04-27 08:41:05.785100512 +0000 UTC m=+16496514.705677824.

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